**D.1. Konza May Sampling**

Input file: C:\Users\huan\Desktop\Konza data\Konza May\Phrqc field pH.pqi

Output file: C:\Users\huan\Desktop\Konza data\Konza May\Phrqc field pH.pqo

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

------------------

Reading data base.

------------------

SOLUTION\_MASTER\_SPECIES

SOLUTION\_SPECIES

PHASES

EXCHANGE\_MASTER\_SPECIES

EXCHANGE\_SPECIES

SURFACE\_MASTER\_SPECIES

SURFACE\_SPECIES

RATES

END

------------------------------------

Reading input data for simulation 1.

------------------------------------

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

SOLUTION\_SPREAD

units mg/l

Description Number pH Temp O(0) Ca K Mg Na Sr B Ba Li Si F N(5) S(6) Cl Alkalinity

mg/L mg/L mg/L mg/L mg/L mg/L mg/L mg/L mg/L mg/L mg/L mg/L mg/L mg/L mg/L as HCO3

L1t1 1 7.3 18.8 4.7 98.13 0.98 20.47 4.34 0.97 0.03 0.12 0.03 6.86 0.60 0.10 34.36 2.20 384

L2t1 2 7.1 18.9 4.8 98.38 0.95 20.36 4.42 0.98 0.03 0.12 0.03 6.95 0.60 0.08 35.09 2.20 385

L3t1 3 7.4 19.9 6.1 97.56 0.95 20.41 4.37 0.96 0.03 0.12 0.03 7.01 0.70 0.07 36.72 2.50 380

SELECTED\_OUTPUT

file Konza May field pH output

reset false

charge\_balance true

percent\_error true

saturation\_indices Calcite CO2(g)

-------------------------------------------

Beginning of initial solution calculations.

-------------------------------------------

Initial solution 1. L1t1

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 6.297e-003 6.297e-003

B 2.777e-006 2.777e-006

Ba 8.742e-007 8.742e-007

Ca 2.450e-003 2.450e-003

Cl 6.209e-005 6.209e-005

F 3.160e-005 3.160e-005

K 2.508e-005 2.508e-005

Li 4.326e-006 4.326e-006

Mg 8.424e-004 8.424e-004

N(5) 7.143e-006 7.143e-006

Na 1.889e-004 1.889e-004

O(0) 2.939e-004 2.939e-004

S(6) 3.579e-004 3.579e-004

Si 1.142e-004 1.142e-004

Sr 1.108e-005 1.108e-005

----------------------------Description of solution----------------------------

pH = 7.300

pe = 4.000

Specific Conductance (uS/cm, 18 oC) = 532

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 1.001e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.957e-003

Total CO2 (mol/kg) = 6.957e-003

Temperature (deg C) = 18.800

Electrical balance (eq) = -2.867e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.16

Iterations = 8

Total H = 1.110192e+002

Total O = 5.552862e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.7866 0.7986

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.365e-007 1.230e-007 -6.865 -6.910 -0.045

H+ 5.482e-008 5.012e-008 -7.261 -7.300 -0.039

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 2.777e-006

H3BO3 2.746e-006 2.752e-006 -5.561 -5.560 0.001

H2BO3- 3.117e-008 2.815e-008 -7.506 -7.551 -0.044

BF(OH)3- 3.100e-011 2.799e-011 -10.509 -10.553 -0.044

BF2(OH)2- 4.585e-015 4.140e-015 -14.339 -14.383 -0.044

BF3OH- 7.725e-021 6.976e-021 -20.112 -20.156 -0.044

BF4- 4.343e-026 3.922e-026 -25.362 -25.407 -0.044

Ba 8.742e-007

Ba+2 7.966e-007 5.344e-007 -6.099 -6.272 -0.173

BaSO4 5.067e-008 5.078e-008 -7.295 -7.294 0.001

BaHCO3+ 2.585e-008 2.334e-008 -7.588 -7.632 -0.044

BaCO3 1.101e-009 1.103e-009 -8.958 -8.957 0.001

BaOH+ 4.001e-013 3.613e-013 -12.398 -12.442 -0.044

C(4) 6.957e-003

HCO3- 6.112e-003 5.538e-003 -2.214 -2.257 -0.043

CO2 6.800e-004 6.815e-004 -3.168 -3.167 0.001

CaHCO3+ 1.073e-004 9.725e-005 -3.969 -4.012 -0.043

MgHCO3+ 3.716e-005 3.355e-005 -4.430 -4.474 -0.044

CaCO3 1.042e-005 1.044e-005 -4.982 -4.981 0.001

CO3-2 6.716e-006 4.525e-006 -5.173 -5.344 -0.171

MgCO3 2.077e-006 2.081e-006 -5.683 -5.682 0.001

NaHCO3 5.285e-007 5.297e-007 -6.277 -6.276 0.001

SrHCO3+ 5.253e-007 4.760e-007 -6.280 -6.322 -0.043

BaHCO3+ 2.585e-008 2.334e-008 -7.588 -7.632 -0.044

SrCO3 1.667e-008 1.671e-008 -7.778 -7.777 0.001

NaCO3- 1.153e-008 1.042e-008 -7.938 -7.982 -0.044

BaCO3 1.101e-009 1.103e-009 -8.958 -8.957 0.001

Ca 2.450e-003

Ca+2 2.277e-003 1.533e-003 -2.643 -2.814 -0.172

CaHCO3+ 1.073e-004 9.725e-005 -3.969 -4.012 -0.043

CaSO4 5.455e-005 5.468e-005 -4.263 -4.262 0.001

CaCO3 1.042e-005 1.044e-005 -4.982 -4.981 0.001

CaF+ 3.484e-007 3.146e-007 -6.458 -6.502 -0.044

CaOH+ 5.622e-009 5.077e-009 -8.250 -8.294 -0.044

CaHSO4+ 1.653e-011 1.493e-011 -10.782 -10.826 -0.044

Cl 6.209e-005

Cl- 6.209e-005 5.596e-005 -4.207 -4.252 -0.045

F 3.160e-005

F- 3.030e-005 2.730e-005 -4.519 -4.564 -0.045

MgF+ 9.444e-007 8.527e-007 -6.025 -6.069 -0.044

CaF+ 3.484e-007 3.146e-007 -6.458 -6.502 -0.044

NaF 2.666e-009 2.673e-009 -8.574 -8.573 0.001

HF 1.834e-009 1.838e-009 -8.737 -8.736 0.001

BF(OH)3- 3.100e-011 2.799e-011 -10.509 -10.553 -0.044

HF2- 2.023e-013 1.826e-013 -12.694 -12.738 -0.044

BF2(OH)2- 4.585e-015 4.140e-015 -14.339 -14.383 -0.044

BF3OH- 7.725e-021 6.976e-021 -20.112 -20.156 -0.044

BF4- 4.343e-026 3.922e-026 -25.362 -25.407 -0.044

SiF6-2 1.218e-030 8.099e-031 -29.914 -30.092 -0.177

H(0) 3.779e-026

H2 1.890e-026 1.894e-026 -25.724 -25.723 0.001

K 2.508e-005

K+ 2.505e-005 2.258e-005 -4.601 -4.646 -0.045

KSO4- 2.982e-008 2.693e-008 -7.525 -7.570 -0.044

KOH 1.558e-012 1.562e-012 -11.807 -11.806 0.001

Li 4.326e-006

Li+ 4.322e-006 3.922e-006 -5.364 -5.406 -0.042

LiSO4- 3.595e-009 3.246e-009 -8.444 -8.489 -0.044

LiOH 1.788e-012 1.793e-012 -11.748 -11.747 0.001

Mg 8.424e-004

Mg+2 7.823e-004 5.302e-004 -3.107 -3.276 -0.169

MgHCO3+ 3.716e-005 3.355e-005 -4.430 -4.474 -0.044

MgSO4 1.997e-005 2.002e-005 -4.700 -4.699 0.001

MgCO3 2.077e-006 2.081e-006 -5.683 -5.682 0.001

MgF+ 9.444e-007 8.527e-007 -6.025 -6.069 -0.044

MgOH+ 2.401e-008 2.168e-008 -7.620 -7.664 -0.044

N(5) 7.143e-006

NO3- 7.143e-006 6.427e-006 -5.146 -5.192 -0.046

Na 1.889e-004

Na+ 1.882e-004 1.701e-004 -3.725 -3.769 -0.044

NaHCO3 5.285e-007 5.297e-007 -6.277 -6.276 0.001

NaSO4- 1.720e-007 1.553e-007 -6.765 -6.809 -0.044

NaCO3- 1.153e-008 1.042e-008 -7.938 -7.982 -0.044

NaF 2.666e-009 2.673e-009 -8.574 -8.573 0.001

NaOH 2.237e-011 2.242e-011 -10.650 -10.649 0.001

O(0) 2.939e-004

O2 1.470e-004 1.473e-004 -3.833 -3.832 0.001

S(6) 3.579e-004

SO4-2 2.829e-004 1.896e-004 -3.548 -3.722 -0.174

CaSO4 5.455e-005 5.468e-005 -4.263 -4.262 0.001

MgSO4 1.997e-005 2.002e-005 -4.700 -4.699 0.001

SrSO4 2.378e-007 2.384e-007 -6.624 -6.623 0.001

NaSO4- 1.720e-007 1.553e-007 -6.765 -6.809 -0.044

BaSO4 5.067e-008 5.078e-008 -7.295 -7.294 0.001

KSO4- 2.982e-008 2.693e-008 -7.525 -7.570 -0.044

LiSO4- 3.595e-009 3.246e-009 -8.444 -8.489 -0.044

HSO4- 8.968e-010 8.098e-010 -9.047 -9.092 -0.044

CaHSO4+ 1.653e-011 1.493e-011 -10.782 -10.826 -0.044

Si 1.142e-004

H4SiO4 1.139e-004 1.142e-004 -3.943 -3.942 0.001

H3SiO4- 2.972e-007 2.684e-007 -6.527 -6.571 -0.044

H2SiO4-2 3.604e-013 2.396e-013 -12.443 -12.621 -0.177

SiF6-2 1.218e-030 8.099e-031 -29.914 -30.092 -0.177

Sr 1.108e-005

Sr+2 1.030e-005 6.947e-006 -4.987 -5.158 -0.171

SrHCO3+ 5.253e-007 4.760e-007 -6.280 -6.322 -0.043

SrSO4 2.378e-007 2.384e-007 -6.624 -6.623 0.001

SrCO3 1.667e-008 1.671e-008 -7.778 -7.777 0.001

SrOH+ 7.854e-012 7.108e-012 -11.105 -11.148 -0.043

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.20 -6.54 -4.34 CaSO4

Aragonite 0.14 -8.16 -8.30 CaCO3

Barite 0.08 -9.99 -10.07 BaSO4

Calcite 0.29 -8.16 -8.45 CaCO3

Celestite -2.26 -8.88 -6.62 SrSO4

Chalcedony -0.32 -3.94 -3.62 SiO2

Chrysotile -6.90 26.09 32.99 Mg3Si2O5(OH)4

CO2(g) -1.78 -3.17 -1.39 CO2

Dolomite 0.16 -16.78 -16.94 CaMg(CO3)2

Fluorite -1.27 -11.94 -10.68 CaF2

Gypsum -1.96 -6.54 -4.58 CaSO4:2H2O

H2(g) -22.60 -25.72 -3.12 H2

H2O(g) -1.67 -0.00 1.67 H2O

Halite -9.59 -8.02 1.57 NaCl

O2(g) -0.99 -3.83 -2.84 O2

Quartz 0.13 -3.94 -4.07 SiO2

Sepiolite -5.10 10.82 15.93 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -7.84 10.82 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.18 -3.94 -2.76 SiO2

Strontianite -1.23 -10.50 -9.27 SrCO3

Talc -3.92 18.20 22.12 Mg3Si4O10(OH)2

Witherite -3.04 -11.62 -8.58 BaCO3

Initial solution 2. L2t1

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 6.313e-003 6.313e-003

B 2.777e-006 2.777e-006

Ba 8.742e-007 8.742e-007

Ca 2.456e-003 2.456e-003

Cl 6.209e-005 6.209e-005

F 3.160e-005 3.160e-005

K 2.431e-005 2.431e-005

Li 4.326e-006 4.326e-006

Mg 8.379e-004 8.379e-004

N(5) 5.715e-006 5.715e-006

Na 1.924e-004 1.924e-004

O(0) 3.002e-004 3.002e-004

S(6) 3.655e-004 3.655e-004

Si 1.157e-004 1.157e-004

Sr 1.119e-005 1.119e-005

----------------------------Description of solution----------------------------

pH = 7.100

pe = 4.000

Specific Conductance (uS/cm, 18 oC) = 535

Density (g/cm3) = 0.99888

Activity of water = 1.000

Ionic strength = 1.004e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.382e-003

Total CO2 (mol/kg) = 7.382e-003

Temperature (deg C) = 18.900

Electrical balance (eq) = -3.105e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.33

Iterations = 9

Total H = 1.110192e+002

Total O = 5.552953e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9803 0.8101

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

H+ 8.690e-008 7.943e-008 -7.061 -7.100 -0.039

OH- 8.684e-008 7.824e-008 -7.061 -7.107 -0.045

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 2.777e-006

H3BO3 2.757e-006 2.763e-006 -5.560 -5.559 0.001

H2BO3- 1.979e-008 1.787e-008 -7.704 -7.748 -0.044

BF(OH)3- 3.117e-011 2.814e-011 -10.506 -10.551 -0.044

BF2(OH)2- 7.303e-015 6.593e-015 -14.137 -14.181 -0.044

BF3OH- 1.946e-020 1.757e-020 -19.711 -19.755 -0.044

BF4- 1.734e-025 1.565e-025 -24.761 -24.805 -0.044

Ba 8.742e-007

Ba+2 7.959e-007 5.336e-007 -6.099 -6.273 -0.174

BaSO4 5.162e-008 5.174e-008 -7.287 -7.286 0.001

BaHCO3+ 2.602e-008 2.349e-008 -7.585 -7.629 -0.044

BaCO3 6.997e-010 7.014e-010 -9.155 -9.154 0.001

BaOH+ 2.521e-013 2.276e-013 -12.598 -12.643 -0.044

C(4) 7.382e-003

HCO3- 6.142e-003 5.564e-003 -2.212 -2.255 -0.043

CO2 1.081e-003 1.084e-003 -2.966 -2.965 0.001

CaHCO3+ 1.084e-004 9.817e-005 -3.965 -4.008 -0.043

MgHCO3+ 3.714e-005 3.353e-005 -4.430 -4.475 -0.044

CaCO3 6.650e-006 6.665e-006 -5.177 -5.176 0.001

CO3-2 4.270e-006 2.876e-006 -5.370 -5.541 -0.172

MgCO3 1.314e-006 1.317e-006 -5.881 -5.880 0.001

NaHCO3 5.407e-007 5.419e-007 -6.267 -6.266 0.001

SrHCO3+ 5.347e-007 4.844e-007 -6.272 -6.315 -0.043

BaHCO3+ 2.602e-008 2.349e-008 -7.585 -7.629 -0.044

SrCO3 1.073e-008 1.075e-008 -7.970 -7.969 0.001

NaCO3- 7.504e-009 6.775e-009 -8.125 -8.169 -0.044

BaCO3 6.997e-010 7.014e-010 -9.155 -9.154 0.001

Ca 2.456e-003

Ca+2 2.285e-003 1.538e-003 -2.641 -2.813 -0.172

CaHCO3+ 1.084e-004 9.817e-005 -3.965 -4.008 -0.043

CaSO4 5.587e-005 5.600e-005 -4.253 -4.252 0.001

CaCO3 6.650e-006 6.665e-006 -5.177 -5.176 0.001

CaF+ 3.502e-007 3.162e-007 -6.456 -6.500 -0.044

CaOH+ 3.558e-009 3.212e-009 -8.449 -8.493 -0.044

CaHSO4+ 2.687e-011 2.426e-011 -10.571 -10.615 -0.044

Cl 6.209e-005

Cl- 6.209e-005 5.596e-005 -4.207 -4.252 -0.045

F 3.160e-005

F- 3.030e-005 2.730e-005 -4.519 -4.564 -0.045

MgF+ 9.408e-007 8.493e-007 -6.027 -6.071 -0.044

CaF+ 3.502e-007 3.162e-007 -6.456 -6.500 -0.044

HF 2.911e-009 2.918e-009 -8.536 -8.535 0.001

NaF 2.715e-009 2.721e-009 -8.566 -8.565 0.001

BF(OH)3- 3.117e-011 2.814e-011 -10.506 -10.551 -0.044

HF2- 3.214e-013 2.902e-013 -12.493 -12.537 -0.044

BF2(OH)2- 7.303e-015 6.593e-015 -14.137 -14.181 -0.044

BF3OH- 1.946e-020 1.757e-020 -19.711 -19.755 -0.044

BF4- 1.734e-025 1.565e-025 -24.761 -24.805 -0.044

SiF6-2 7.720e-030 5.129e-030 -29.112 -29.290 -0.178

H(0) 9.483e-026

H2 4.742e-026 4.753e-026 -25.324 -25.323 0.001

K 2.431e-005

K+ 2.428e-005 2.188e-005 -4.615 -4.660 -0.045

KSO4- 2.955e-008 2.668e-008 -7.529 -7.574 -0.044

KOH 9.528e-013 9.550e-013 -12.021 -12.020 0.001

Li 4.326e-006

Li+ 4.322e-006 3.922e-006 -5.364 -5.407 -0.042

LiSO4- 3.668e-009 3.312e-009 -8.436 -8.480 -0.044

LiOH 1.128e-012 1.131e-012 -11.948 -11.947 0.001

Mg 8.379e-004

Mg+2 7.782e-004 5.271e-004 -3.109 -3.278 -0.169

MgHCO3+ 3.714e-005 3.353e-005 -4.430 -4.475 -0.044

MgSO4 2.031e-005 2.036e-005 -4.692 -4.691 0.001

MgCO3 1.314e-006 1.317e-006 -5.881 -5.880 0.001

MgF+ 9.408e-007 8.493e-007 -6.027 -6.071 -0.044

MgOH+ 1.521e-008 1.373e-008 -7.818 -7.862 -0.044

N(5) 5.715e-006

NO3- 5.715e-006 5.140e-006 -5.243 -5.289 -0.046

Na 1.924e-004

Na+ 1.916e-004 1.732e-004 -3.718 -3.761 -0.044

NaHCO3 5.407e-007 5.419e-007 -6.267 -6.266 0.001

NaSO4- 1.788e-007 1.614e-007 -6.748 -6.792 -0.044

NaCO3- 7.504e-009 6.775e-009 -8.125 -8.169 -0.044

NaF 2.715e-009 2.721e-009 -8.566 -8.565 0.001

NaOH 1.437e-011 1.440e-011 -10.843 -10.842 0.001

O(0) 3.002e-004

O2 1.501e-004 1.504e-004 -3.824 -3.823 0.001

S(6) 3.655e-004

SO4-2 2.888e-004 1.935e-004 -3.539 -3.713 -0.174

CaSO4 5.587e-005 5.600e-005 -4.253 -4.252 0.001

MgSO4 2.031e-005 2.036e-005 -4.692 -4.691 0.001

SrSO4 2.453e-007 2.458e-007 -6.610 -6.609 0.001

NaSO4- 1.788e-007 1.614e-007 -6.748 -6.792 -0.044

BaSO4 5.162e-008 5.174e-008 -7.287 -7.286 0.001

KSO4- 2.955e-008 2.668e-008 -7.529 -7.574 -0.044

LiSO4- 3.668e-009 3.312e-009 -8.436 -8.480 -0.044

HSO4- 1.453e-009 1.312e-009 -8.838 -8.882 -0.044

CaHSO4+ 2.687e-011 2.426e-011 -10.571 -10.615 -0.044

Si 1.157e-004

H4SiO4 1.155e-004 1.158e-004 -3.937 -3.936 0.001

H3SiO4- 1.909e-007 1.724e-007 -6.719 -6.764 -0.044

H2SiO4-2 1.472e-013 9.778e-014 -12.832 -13.010 -0.178

SiF6-2 7.720e-030 5.129e-030 -29.112 -29.290 -0.178

Sr 1.119e-005

Sr+2 1.040e-005 7.013e-006 -4.983 -5.154 -0.171

SrHCO3+ 5.347e-007 4.844e-007 -6.272 -6.315 -0.043

SrSO4 2.453e-007 2.458e-007 -6.610 -6.609 0.001

SrCO3 1.073e-008 1.075e-008 -7.970 -7.969 0.001

SrOH+ 5.003e-012 4.527e-012 -11.301 -11.344 -0.043

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.19 -6.53 -4.34 CaSO4

Aragonite -0.05 -8.35 -8.30 CaCO3

Barite 0.09 -9.99 -10.07 BaSO4

Calcite 0.09 -8.35 -8.45 CaCO3

Celestite -2.25 -8.87 -6.62 SrSO4

Chalcedony -0.31 -3.94 -3.62 SiO2

Chrysotile -8.08 24.89 32.97 Mg3Si2O5(OH)4

CO2(g) -1.57 -2.97 -1.39 CO2

Dolomite -0.23 -17.17 -16.95 CaMg(CO3)2

Fluorite -1.27 -11.94 -10.67 CaF2

Gypsum -1.95 -6.53 -4.58 CaSO4:2H2O

H2(g) -22.20 -25.32 -3.12 H2

H2O(g) -1.67 -0.00 1.67 H2O

Halite -9.58 -8.01 1.57 NaCl

O2(g) -0.98 -3.82 -2.85 O2

Quartz 0.14 -3.94 -4.07 SiO2

Sepiolite -5.89 10.04 15.92 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.62 10.04 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.17 -3.94 -2.76 SiO2

Strontianite -1.43 -10.70 -9.27 SrCO3

Talc -5.09 17.02 22.11 Mg3Si4O10(OH)2

Witherite -3.23 -11.81 -8.58 BaCO3

Initial solution 3. L3t1

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 6.231e-003 6.231e-003

B 2.777e-006 2.777e-006

Ba 8.742e-007 8.742e-007

Ca 2.435e-003 2.435e-003

Cl 7.056e-005 7.056e-005

F 3.687e-005 3.687e-005

K 2.431e-005 2.431e-005

Li 4.326e-006 4.326e-006

Mg 8.400e-004 8.400e-004

N(5) 5.000e-006 5.000e-006

Na 1.902e-004 1.902e-004

O(0) 3.815e-004 3.815e-004

S(6) 3.825e-004 3.825e-004

Si 1.167e-004 1.167e-004

Sr 1.096e-005 1.096e-005

----------------------------Description of solution----------------------------

pH = 7.400

pe = 4.000

Specific Conductance (uS/cm, 19 oC) = 545

Density (g/cm3) = 0.99868

Activity of water = 1.000

Ionic strength = 9.966e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.730e-003

Total CO2 (mol/kg) = 6.730e-003

Temperature (deg C) = 19.900

Electrical balance (eq) = -3.149e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.38

Iterations = 7

Total H = 1.110191e+002

Total O = 5.552828e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.6202 0.7919

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.877e-007 1.692e-007 -6.726 -6.772 -0.045

H+ 4.355e-008 3.981e-008 -7.361 -7.400 -0.039

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 2.777e-006

H3BO3 2.737e-006 2.743e-006 -5.563 -5.562 0.001

H2BO3- 3.994e-008 3.607e-008 -7.399 -7.443 -0.044

BF(OH)3- 3.646e-011 3.293e-011 -10.438 -10.482 -0.044

BF2(OH)2- 4.987e-015 4.503e-015 -14.302 -14.347 -0.044

BF3OH- 7.621e-021 6.882e-021 -20.118 -20.162 -0.044

BF4- 3.962e-026 3.578e-026 -25.402 -25.446 -0.044

Ba 8.742e-007

Ba+2 7.927e-007 5.318e-007 -6.101 -6.274 -0.173

BaSO4 5.380e-008 5.392e-008 -7.269 -7.268 0.001

BaHCO3+ 2.630e-008 2.375e-008 -7.580 -7.624 -0.044

BaCO3 1.428e-009 1.432e-009 -8.845 -8.844 0.001

BaOH+ 5.012e-013 4.526e-013 -12.300 -12.344 -0.044

C(4) 6.730e-003

HCO3- 6.036e-003 5.469e-003 -2.219 -2.262 -0.043

CO2 5.242e-004 5.254e-004 -3.280 -3.279 0.001

CaHCO3+ 1.073e-004 9.720e-005 -3.969 -4.012 -0.043

MgHCO3+ 3.662e-005 3.306e-005 -4.436 -4.481 -0.044

CaCO3 1.340e-005 1.343e-005 -4.873 -4.872 0.001

CO3-2 8.565e-006 5.772e-006 -5.067 -5.239 -0.171

MgCO3 2.678e-006 2.684e-006 -5.572 -5.571 0.001

SrHCO3+ 5.313e-007 4.814e-007 -6.275 -6.317 -0.043

NaHCO3 5.255e-007 5.267e-007 -6.279 -6.278 0.001

BaHCO3+ 2.630e-008 2.375e-008 -7.580 -7.624 -0.044

SrCO3 2.167e-008 2.172e-008 -7.664 -7.663 0.001

NaCO3- 1.569e-008 1.417e-008 -7.804 -7.849 -0.044

BaCO3 1.428e-009 1.432e-009 -8.845 -8.844 0.001

Ca 2.435e-003

Ca+2 2.256e-003 1.519e-003 -2.647 -2.818 -0.172

CaHCO3+ 1.073e-004 9.720e-005 -3.969 -4.012 -0.043

CaSO4 5.830e-005 5.843e-005 -4.234 -4.233 0.001

CaCO3 1.340e-005 1.343e-005 -4.873 -4.872 0.001

CaF+ 4.134e-007 3.733e-007 -6.384 -6.428 -0.044

CaOH+ 7.013e-009 6.333e-009 -8.154 -8.198 -0.044

CaHSO4+ 1.421e-011 1.283e-011 -10.848 -10.892 -0.044

Cl 7.056e-005

Cl- 7.056e-005 6.360e-005 -4.151 -4.197 -0.045

F 3.687e-005

F- 3.533e-005 3.183e-005 -4.452 -4.497 -0.045

MgF+ 1.118e-006 1.009e-006 -5.952 -5.996 -0.044

CaF+ 4.134e-007 3.733e-007 -6.384 -6.428 -0.044

NaF 3.130e-009 3.137e-009 -8.504 -8.503 0.001

HF 1.732e-009 1.736e-009 -8.762 -8.761 0.001

BF(OH)3- 3.646e-011 3.293e-011 -10.438 -10.482 -0.044

HF2- 2.250e-013 2.031e-013 -12.648 -12.692 -0.044

BF2(OH)2- 4.987e-015 4.503e-015 -14.302 -14.347 -0.044

BF3OH- 7.621e-021 6.882e-021 -20.118 -20.162 -0.044

BF4- 3.962e-026 3.578e-026 -25.402 -25.446 -0.044

SiF6-2 1.120e-030 7.445e-031 -29.951 -30.128 -0.177

H(0) 2.358e-026

H2 1.179e-026 1.182e-026 -25.929 -25.928 0.001

K 2.431e-005

K+ 2.428e-005 2.188e-005 -4.615 -4.660 -0.045

KSO4- 3.147e-008 2.841e-008 -7.502 -7.546 -0.044

KOH 1.901e-012 1.906e-012 -11.721 -11.720 0.001

Li 4.326e-006

Li+ 4.322e-006 3.922e-006 -5.364 -5.406 -0.042

LiSO4- 3.836e-009 3.464e-009 -8.416 -8.460 -0.044

LiOH 2.251e-012 2.257e-012 -11.648 -11.647 0.001

Mg 8.400e-004

Mg+2 7.777e-004 5.271e-004 -3.109 -3.278 -0.169

MgHCO3+ 3.662e-005 3.306e-005 -4.436 -4.481 -0.044

MgSO4 2.182e-005 2.187e-005 -4.661 -4.660 0.001

MgCO3 2.678e-006 2.684e-006 -5.572 -5.571 0.001

MgF+ 1.118e-006 1.009e-006 -5.952 -5.996 -0.044

MgOH+ 3.332e-008 3.008e-008 -7.477 -7.522 -0.044

N(5) 5.000e-006

NO3- 5.000e-006 4.499e-006 -5.301 -5.347 -0.046

Na 1.902e-004

Na+ 1.895e-004 1.713e-004 -3.722 -3.766 -0.044

NaHCO3 5.255e-007 5.267e-007 -6.279 -6.278 0.001

NaSO4- 1.861e-007 1.680e-007 -6.730 -6.775 -0.044

NaCO3- 1.569e-008 1.417e-008 -7.804 -7.849 -0.044

NaF 3.130e-009 3.137e-009 -8.504 -8.503 0.001

NaOH 2.835e-011 2.842e-011 -10.547 -10.546 0.001

O(0) 3.815e-004

O2 1.907e-004 1.912e-004 -3.720 -3.719 0.001

S(6) 3.825e-004

SO4-2 3.018e-004 2.023e-004 -3.520 -3.694 -0.174

CaSO4 5.830e-005 5.843e-005 -4.234 -4.233 0.001

MgSO4 2.182e-005 2.187e-005 -4.661 -4.660 0.001

SrSO4 2.537e-007 2.543e-007 -6.596 -6.595 0.001

NaSO4- 1.861e-007 1.680e-007 -6.730 -6.775 -0.044

BaSO4 5.380e-008 5.392e-008 -7.269 -7.268 0.001

KSO4- 3.147e-008 2.841e-008 -7.502 -7.546 -0.044

LiSO4- 3.836e-009 3.464e-009 -8.416 -8.460 -0.044

HSO4- 7.777e-010 7.022e-010 -9.109 -9.154 -0.044

CaHSO4+ 1.421e-011 1.283e-011 -10.848 -10.892 -0.044

Si 1.167e-004

H4SiO4 1.163e-004 1.166e-004 -3.934 -3.933 0.001

H3SiO4- 3.981e-007 3.595e-007 -6.400 -6.444 -0.044

H2SiO4-2 6.561e-013 4.362e-013 -12.183 -12.360 -0.177

SiF6-2 1.120e-030 7.445e-031 -29.951 -30.128 -0.177

Sr 1.096e-005

Sr+2 1.016e-005 6.852e-006 -4.993 -5.164 -0.171

SrHCO3+ 5.313e-007 4.814e-007 -6.275 -6.317 -0.043

SrSO4 2.537e-007 2.543e-007 -6.596 -6.595 0.001

SrCO3 2.167e-008 2.172e-008 -7.664 -7.663 0.001

SrOH+ 9.752e-012 8.826e-012 -11.011 -11.054 -0.043

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.17 -6.51 -4.34 CaSO4

Aragonite 0.25 -8.06 -8.31 CaCO3

Barite 0.09 -9.97 -10.05 BaSO4

Calcite 0.40 -8.06 -8.45 CaCO3

Celestite -2.24 -8.86 -6.62 SrSO4

Chalcedony -0.32 -3.93 -3.61 SiO2

Chrysotile -6.14 26.70 32.84 Mg3Si2O5(OH)4

CO2(g) -1.87 -3.28 -1.41 CO2

Dolomite 0.40 -16.57 -16.97 CaMg(CO3)2

Fluorite -1.15 -11.81 -10.66 CaF2

Gypsum -1.93 -6.51 -4.58 CaSO4:2H2O

H2(g) -22.80 -25.93 -3.13 H2

H2O(g) -1.64 -0.00 1.64 H2O

Halite -9.53 -7.96 1.57 NaCl

O2(g) -0.87 -3.72 -2.85 O2

Quartz 0.12 -3.93 -4.06 SiO2

Sepiolite -4.65 11.24 15.90 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -7.42 11.24 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.18 -3.93 -2.75 SiO2

Strontianite -1.13 -10.40 -9.27 SrCO3

Talc -3.16 18.83 21.99 Mg3Si4O10(OH)2

Witherite -2.94 -11.51 -8.58 BaCO3

------------------

End of simulation.

------------------

------------------------------------

Reading input data for simulation 2.

------------------------------------

-----------

End of run.

**D.2. Maolan Sampling**

Input file: C:\Users\huan\Desktop\Maolan Spring.pqi

Output file: C:\Users\huan\Desktop\Maolan Spring.pqo

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

------------------

Reading data base.

------------------

SOLUTION\_MASTER\_SPECIES

SOLUTION\_SPECIES

PHASES

EXCHANGE\_MASTER\_SPECIES

EXCHANGE\_SPECIES

SURFACE\_MASTER\_SPECIES

SURFACE\_SPECIES

RATES

END

------------------------------------

Reading input data for simulation 1.

------------------------------------

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

SOLUTION\_SPREAD

units mg/l

Description Number pH Temp O(0) Ca K Mg Na S(6) Cl Alkalinity

mg/L mg/L mg/L mg/L mg/L mg/L mg/L mg/L as HCO3

29/8/2012 11:54:20 1 7.28 17.7 6.68 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

29/8/2012 12:09:20 2 7.23 17.8 6.34 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

29/8/2012 12:24:20 3 7.24 17.7 6.8 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

29/8/2012 12:39:20 4 7.23 17.7 6.8 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

29/8/2012 12:54:20 5 7.22 17.7 6.7 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

29/8/2012 13:09:20 6 7.23 17.7 6.63 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

29/8/2012 13:24:20 7 7.2 17.7 6.46 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

29/8/2012 13:39:20 8 7.16 17.7 6.55 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

29/8/2012 13:54:20 9 7.22 17.6 6.73 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

29/8/2012 14:09:20 10 7.22 17.6 6.44 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

29/8/2012 14:24:20 11 7.21 17.6 6.54 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

29/8/2012 14:39:20 12 7.22 17.6 6.7 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

29/8/2012 14:54:20 13 7.2 17.6 6.63 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

29/8/2012 15:09:20 14 7.2 17.6 6.42 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 15:24:20 15 7.21 17.5 6.37 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 15:39:20 16 7.16 17.5 6.45 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 15:54:20 17 7.2 17.5 6.3 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 16:09:20 18 7.2 17.5 6.21 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 16:24:20 19 7.16 17.5 6.2 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 16:39:20 20 7.2 17.5 6 53.82 0.13 12.60 0.23 11.07999992 2.029999971 224.61

29/8/2012 16:54:20 21 7.19 17.5 6.04 53.82 0.13 12.60 0.23 11.07999992 2.029999971 224.61

29/8/2012 17:09:20 22 7.21 17.5 5.91 53.82 0.13 12.60 0.23 11.07999992 2.029999971 224.61

29/8/2012 17:24:20 23 7.22 17.5 6.09 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 17:39:20 24 7.2 17.5 6.41 53.82 0.13 12.60 0.23 11.07999992 2.029999971 224.61

29/8/2012 17:54:20 25 7.22 17.5 6.12 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 18:09:20 26 7.21 17.5 6.24 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 18:24:20 27 7.2 17.5 6.1 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 18:39:20 28 7.19 17.5 6 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 18:54:20 29 7.2 17.5 6.19 53.82 0.13 12.60 0.23 11.07999992 2.029999971 224.61

29/8/2012 19:09:20 30 7.22 17.5 6.34 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 19:24:20 31 7.2 17.5 6.12 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 19:39:20 32 7.11 17.5 6.23 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 19:54:20 33 7.19 17.5 6.7 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 20:09:20 34 7.21 17.5 6.08 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 20:24:20 35 7.2 17.5 6.58 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 20:39:20 36 7.19 17.5 6.16 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 20:54:20 37 7.19 17.5 6.25 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 21:09:20 38 7.19 17.5 6.4 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 21:24:20 39 7.27 17.5 6.67 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 21:39:20 40 7.19 17.5 6.06 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 21:54:20 41 7.16 17.5 6.01 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 22:09:20 42 7.2 17.5 5.99 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 22:24:20 43 7.24 17.4 6.47 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 22:39:20 44 7.13 17.5 6.08 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 22:54:20 45 7.22 17.5 6.03 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 23:09:20 46 7.22 17.4 6.04 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 23:24:20 47 7.22 17.5 6.56 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 23:39:20 48 7.21 17.4 6.79 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 23:54:20 49 7.22 17.5 6.44 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 00:09:20 50 7.21 17.4 7.05 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 00:24:20 51 7.21 17.5 5.93 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 00:39:20 52 7.21 17.5 5.94 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 00:54:20 53 7.21 17.4 6.74 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 01:09:20 54 7.22 17.5 6.31 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 01:24:20 55 7.21 17.5 6.05 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 01:39:20 56 7.22 17.5 6.62 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 01:54:20 57 7.21 17.5 6.17 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 02:09:20 58 7.22 17.5 5.94 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 02:24:20 59 7.22 17.4 6.75 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 02:39:20 60 7.21 17.5 6.79 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 02:54:20 61 7.22 17.4 6.11 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 03:09:20 62 7.22 17.4 6.12 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 03:24:20 63 7.22 17.5 6.54 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 03:39:20 64 7.14 17.5 6.1 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 03:54:20 65 7.22 17.5 6.47 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 04:09:20 66 7.22 17.5 6.5 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 04:24:20 67 7.22 17.5 6.83 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 04:39:20 68 7.22 17.5 6.9 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 04:54:20 69 7.23 17.5 6.41 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 05:09:20 70 7.17 17.5 6.19 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 05:24:20 71 7.2 17.5 6.43 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 05:39:20 72 7.16 17.5 6.41 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 05:54:20 73 7.25 17.5 6.43 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 06:09:20 74 7.24 17.5 6.7 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 06:24:20 75 7.22 17.5 6.33 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 06:39:20 76 7.24 17.5 6.64 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 06:54:20 77 7.2 17.5 5.91 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 07:09:20 78 7.21 17.5 6.13 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 07:24:20 79 7.22 17.5 6.37 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 07:39:20 80 7.23 17.5 6.21 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 07:54:20 81 7.24 17.5 5.84 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 08:09:20 82 7.23 17.5 6.3 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 08:24:20 83 7.24 17.5 6.18 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 08:39:20 84 7.24 17.5 5.96 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 08:54:20 85 7.23 17.5 5.94 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 09:09:20 86 7.23 17.5 6.63 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 09:24:20 87 7.23 17.5 6.64 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 09:39:20 88 7.23 17.5 6.44 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 09:54:20 89 7.23 17.5 6.13 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 10:09:20 90 7.23 17.5 5.79 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 10:24:20 91 7.23 17.5 6.4 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 10:39:20 92 7.23 17.5 6.04 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 10:54:20 93 7.23 17.6 6.05 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 11:09:20 94 7.22 17.6 6.23 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 11:24:20 95 7.22 17.7 6.24 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 11:39:20 96 7.22 17.6 6.45 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 11:54:20 97 7.22 17.7 6.36 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 12:09:20 98 7.22 17.7 6.11 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 12:24:20 99 7.22 17.7 6.49 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 12:39:20 100 7.22 17.8 6.58 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

30/8/2012 12:54:20 101 7.23 17.8 6.73 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 13:09:20 102 7.23 17.8 6.72 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

30/8/2012 13:24:20 103 7.23 17.7 6.29 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 13:39:20 104 7.23 17.8 6.78 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 13:54:20 105 7.24 17.8 6.32 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 14:09:20 106 7.23 17.8 6.46 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 14:24:20 107 7.24 17.8 6.37 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 14:54:20 108 7.23 17.8 6.08 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 15:09:20 109 7.23 17.9 6.47 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 15:24:20 110 7.23 17.8 5.83 52.92 0.13 12.60 0.23 11.07999992 2.029999971 220.83

30/8/2012 15:39:20 111 7.23 17.8 6.14 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 15:54:20 112 7.23 17.8 6.3 53.07 0.13 12.60 0.23 11.07999992 2.029999971 221.47

30/8/2012 16:09:20 113 7.23 17.7 6.33 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 16:24:20 114 7.23 17.7 5.87 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 16:39:20 115 7.23 17.7 6.31 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 16:54:20 116 7.22 17.6 6.36 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 17:09:20 117 7.2 17.6 6.42 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 17:24:20 118 7.22 17.6 6.53 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 17:39:20 119 7.22 17.6 6.39 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 17:54:20 120 7.2 17.6 6.17 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

SELECTED\_OUTPUT

file C:\Users\huan\Desktop\selected output spring.sel

reset false

saturation\_indices Calcite CO2(g)

-------------------------------------------

Beginning of initial solution calculations.

-------------------------------------------

Initial solution 1. 29/8/2012 11:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.176e-004 4.176e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.280

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.607e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.078e-003

Total CO2 (mol/kg) = 4.078e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.02

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551890e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9400 0.8044

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.164e-007 1.074e-007 -6.934 -6.969 -0.035

H+ 5.635e-008 5.248e-008 -7.249 -7.280 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.078e-003

HCO3- 3.583e-003 3.319e-003 -2.446 -2.479 -0.033

CO2 4.349e-004 4.355e-004 -3.362 -3.361 0.001

CaHCO3+ 3.773e-005 3.494e-005 -4.423 -4.457 -0.033

MgHCO3+ 1.502e-005 1.389e-005 -4.823 -4.857 -0.034

CaCO3 3.508e-006 3.513e-006 -5.455 -5.454 0.001

CO3-2 3.428e-006 2.523e-006 -5.465 -5.598 -0.133

MgCO3 7.895e-007 7.905e-007 -6.103 -6.102 0.001

NaHCO3 1.721e-008 1.724e-008 -7.764 -7.764 0.001

NaCO3- 3.219e-010 2.975e-010 -9.492 -9.527 -0.034

Ca 1.332e-003

Ca+2 1.278e-003 9.403e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.773e-005 3.494e-005 -4.423 -4.457 -0.033

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

CaCO3 3.508e-006 3.513e-006 -5.455 -5.454 0.001

CaOH+ 3.217e-009 2.973e-009 -8.493 -8.527 -0.034

CaHSO4+ 3.835e-012 3.545e-012 -11.416 -11.450 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 4.196e-026

H2 2.098e-026 2.101e-026 -25.678 -25.678 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

KOH 2.025e-013 2.028e-013 -12.694 -12.693 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.502e-005 1.389e-005 -4.823 -4.857 -0.034

MgSO4 5.087e-006 5.093e-006 -5.294 -5.293 0.001

MgCO3 7.895e-007 7.905e-007 -6.103 -6.102 0.001

MgOH+ 1.399e-008 1.293e-008 -7.854 -7.888 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.721e-008 1.724e-008 -7.764 -7.764 0.001

NaSO4- 3.426e-009 3.166e-009 -8.465 -8.499 -0.034

NaCO3- 3.219e-010 2.975e-010 -9.492 -9.527 -0.034

NaOH 1.161e-012 1.163e-012 -11.935 -11.935 0.001

O(0) 4.176e-004

O2 2.088e-004 2.091e-004 -3.680 -3.680 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.172e-005 -4.010 -4.144 -0.135

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

MgSO4 5.087e-006 5.093e-006 -5.294 -5.293 0.001

NaSO4- 3.426e-009 3.166e-009 -8.465 -8.499 -0.034

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

HSO4- 3.393e-010 3.136e-010 -9.469 -9.504 -0.034

CaHSO4+ 3.835e-012 3.545e-012 -11.416 -11.450 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.33 -8.62 -8.29 CaCO3

Calcite -0.18 -8.62 -8.44 CaCO3

CO2(g) -1.98 -3.36 -1.38 CO2

Dolomite -0.74 -17.66 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.56 -25.68 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.84 -3.68 -2.84 O2

Initial solution 2. 29/8/2012 12:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.964e-004 3.964e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.608e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.132e-003

Total CO2 (mol/kg) = 4.132e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.02

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551898e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9757 0.8068

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.046e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.322e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.132e-003

HCO3- 3.584e-003 3.320e-003 -2.446 -2.479 -0.033

CO2 4.873e-004 4.880e-004 -3.312 -3.312 0.001

CaHCO3+ 3.783e-005 3.504e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

CaCO3 3.140e-006 3.144e-006 -5.503 -5.502 0.001

CO3-2 3.064e-006 2.255e-006 -5.514 -5.647 -0.133

MgCO3 7.067e-007 7.077e-007 -6.151 -6.150 0.001

NaHCO3 1.722e-008 1.724e-008 -7.764 -7.763 0.001

NaCO3- 2.892e-010 2.673e-010 -9.539 -9.573 -0.034

Ca 1.332e-003

Ca+2 1.278e-003 9.404e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.783e-005 3.504e-005 -4.422 -4.455 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.140e-006 3.144e-006 -5.503 -5.502 0.001

CaOH+ 2.867e-009 2.650e-009 -8.543 -8.577 -0.034

CaHSO4+ 4.311e-012 3.985e-012 -11.365 -11.400 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.471e-009 1.359e-009 -8.832 -8.867 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

MgSO4 5.099e-006 5.106e-006 -5.292 -5.292 0.001

MgCO3 7.067e-007 7.077e-007 -6.151 -6.150 0.001

MgOH+ 1.259e-008 1.163e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.722e-008 1.724e-008 -7.764 -7.763 0.001

NaSO4- 3.427e-009 3.167e-009 -8.465 -8.499 -0.034

NaCO3- 2.892e-010 2.673e-010 -9.539 -9.573 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.964e-004

O2 1.982e-004 1.984e-004 -3.703 -3.702 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.170e-005 -4.010 -4.145 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.099e-006 5.106e-006 -5.292 -5.292 0.001

NaSO4- 3.427e-009 3.167e-009 -8.465 -8.499 -0.034

KSO4- 1.471e-009 1.359e-009 -8.832 -8.867 -0.034

HSO4- 3.813e-010 3.525e-010 -9.419 -9.453 -0.034

CaHSO4+ 4.311e-012 3.985e-012 -11.365 -11.400 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.76 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.87 -3.70 -2.84 O2

Initial solution 3. 29/8/2012 12:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.251e-004 4.251e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.608e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.121e-003

Total CO2 (mol/kg) = 4.121e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.02

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551899e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9820 0.8069

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.061e-007 9.798e-008 -6.974 -7.009 -0.035

H+ 6.178e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.121e-003

HCO3- 3.584e-003 3.320e-003 -2.446 -2.479 -0.033

CO2 4.770e-004 4.776e-004 -3.321 -3.321 0.001

CaHCO3+ 3.775e-005 3.496e-005 -4.423 -4.456 -0.033

MgHCO3+ 1.503e-005 1.389e-005 -4.823 -4.857 -0.034

CaCO3 3.201e-006 3.205e-006 -5.495 -5.494 0.001

CO3-2 3.127e-006 2.302e-006 -5.505 -5.638 -0.133

MgCO3 7.204e-007 7.213e-007 -6.142 -6.142 0.001

NaHCO3 1.722e-008 1.724e-008 -7.764 -7.763 0.001

NaCO3- 2.936e-010 2.714e-010 -9.532 -9.566 -0.034

Ca 1.332e-003

Ca+2 1.279e-003 9.404e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.775e-005 3.496e-005 -4.423 -4.456 -0.033

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

CaCO3 3.201e-006 3.205e-006 -5.495 -5.494 0.001

CaOH+ 2.934e-009 2.712e-009 -8.532 -8.567 -0.034

CaHSO4+ 4.206e-012 3.887e-012 -11.376 -11.410 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 5.045e-026

H2 2.522e-026 2.526e-026 -25.598 -25.598 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.503e-005 1.389e-005 -4.823 -4.857 -0.034

MgSO4 5.087e-006 5.094e-006 -5.294 -5.293 0.001

MgCO3 7.204e-007 7.213e-007 -6.142 -6.142 0.001

MgOH+ 1.276e-008 1.179e-008 -7.894 -7.928 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.722e-008 1.724e-008 -7.764 -7.763 0.001

NaSO4- 3.426e-009 3.166e-009 -8.465 -8.499 -0.034

NaCO3- 2.936e-010 2.714e-010 -9.532 -9.566 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 4.251e-004

O2 2.126e-004 2.128e-004 -3.673 -3.672 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

MgSO4 5.087e-006 5.094e-006 -5.294 -5.293 0.001

NaSO4- 3.426e-009 3.166e-009 -8.465 -8.499 -0.034

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

HSO4- 3.720e-010 3.438e-010 -9.429 -9.464 -0.034

CaHSO4+ 4.206e-012 3.887e-012 -11.376 -11.410 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.38 CO2

Dolomite -0.82 -17.74 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.84 -3.67 -2.84 O2

Initial solution 4. 29/8/2012 12:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.251e-004 4.251e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.608e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.132e-003

Total CO2 (mol/kg) = 4.132e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.02

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551901e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9920 0.8074

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.037e-007 9.575e-008 -6.984 -7.019 -0.035

H+ 6.322e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.132e-003

HCO3- 3.584e-003 3.320e-003 -2.446 -2.479 -0.033

CO2 4.882e-004 4.888e-004 -3.311 -3.311 0.001

CaHCO3+ 3.775e-005 3.497e-005 -4.423 -4.456 -0.033

MgHCO3+ 1.503e-005 1.389e-005 -4.823 -4.857 -0.034

CaCO3 3.129e-006 3.133e-006 -5.505 -5.504 0.001

CO3-2 3.056e-006 2.249e-006 -5.515 -5.648 -0.133

MgCO3 7.040e-007 7.050e-007 -6.152 -6.152 0.001

NaHCO3 1.722e-008 1.724e-008 -7.764 -7.763 0.001

NaCO3- 2.870e-010 2.652e-010 -9.542 -9.576 -0.034

Ca 1.332e-003

Ca+2 1.279e-003 9.405e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.775e-005 3.497e-005 -4.423 -4.456 -0.033

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

CaCO3 3.129e-006 3.133e-006 -5.505 -5.504 0.001

CaOH+ 2.868e-009 2.650e-009 -8.542 -8.577 -0.034

CaHSO4+ 4.304e-012 3.978e-012 -11.366 -11.400 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 5.282e-026

H2 2.641e-026 2.645e-026 -25.578 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.503e-005 1.389e-005 -4.823 -4.857 -0.034

MgSO4 5.087e-006 5.094e-006 -5.294 -5.293 0.001

MgCO3 7.040e-007 7.050e-007 -6.152 -6.152 0.001

MgOH+ 1.247e-008 1.152e-008 -7.904 -7.938 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.722e-008 1.724e-008 -7.764 -7.763 0.001

NaSO4- 3.425e-009 3.166e-009 -8.465 -8.499 -0.034

NaCO3- 2.870e-010 2.652e-010 -9.542 -9.576 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.251e-004

O2 2.126e-004 2.128e-004 -3.673 -3.672 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

MgSO4 5.087e-006 5.094e-006 -5.294 -5.293 0.001

NaSO4- 3.425e-009 3.166e-009 -8.465 -8.499 -0.034

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

HSO4- 3.807e-010 3.518e-010 -9.419 -9.454 -0.034

CaHSO4+ 4.304e-012 3.978e-012 -11.366 -11.400 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.76 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.84 -3.67 -2.84 O2

Initial solution 5. 29/8/2012 12:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.189e-004 4.189e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.608e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.144e-003

Total CO2 (mol/kg) = 4.144e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.01

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551903e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0004 0.8079

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.014e-007 9.357e-008 -6.994 -7.029 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.144e-003

HCO3- 3.585e-003 3.320e-003 -2.446 -2.479 -0.033

CO2 4.996e-004 5.002e-004 -3.301 -3.301 0.001

CaHCO3+ 3.776e-005 3.497e-005 -4.423 -4.456 -0.033

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

CaCO3 3.058e-006 3.062e-006 -5.515 -5.514 0.001

CO3-2 2.987e-006 2.198e-006 -5.525 -5.658 -0.133

MgCO3 6.881e-007 6.890e-007 -6.162 -6.162 0.001

NaHCO3 1.722e-008 1.725e-008 -7.764 -7.763 0.001

NaCO3- 2.805e-010 2.592e-010 -9.552 -9.586 -0.034

Ca 1.332e-003

Ca+2 1.279e-003 9.405e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.776e-005 3.497e-005 -4.423 -4.456 -0.033

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

CaCO3 3.058e-006 3.062e-006 -5.515 -5.514 0.001

CaOH+ 2.802e-009 2.590e-009 -8.552 -8.587 -0.034

CaHSO4+ 4.405e-012 4.071e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 5.531e-026

H2 2.766e-026 2.769e-026 -25.558 -25.558 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

MgSO4 5.087e-006 5.094e-006 -5.294 -5.293 0.001

MgCO3 6.881e-007 6.890e-007 -6.162 -6.162 0.001

MgOH+ 1.219e-008 1.126e-008 -7.914 -7.948 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.722e-008 1.725e-008 -7.764 -7.763 0.001

NaSO4- 3.425e-009 3.166e-009 -8.465 -8.499 -0.034

NaCO3- 2.805e-010 2.592e-010 -9.552 -9.586 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.189e-004

O2 2.094e-004 2.097e-004 -3.679 -3.678 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

MgSO4 5.087e-006 5.094e-006 -5.294 -5.293 0.001

NaSO4- 3.425e-009 3.166e-009 -8.465 -8.499 -0.034

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

HSO4- 3.895e-010 3.600e-010 -9.409 -9.444 -0.034

CaHSO4+ 4.405e-012 4.071e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.84 -3.68 -2.84 O2

Initial solution 6. 29/8/2012 13:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.145e-004 4.145e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.144e-003

Total CO2 (mol/kg) = 4.144e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9892 0.8073

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.037e-007 9.575e-008 -6.984 -7.019 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.144e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.895e-004 4.902e-004 -3.310 -3.310 0.001

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CO3-2 3.066e-006 2.256e-006 -5.513 -5.647 -0.133

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.282e-026

H2 2.641e-026 2.645e-026 -25.578 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

MgOH+ 1.247e-008 1.152e-008 -7.904 -7.939 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.145e-004

O2 2.073e-004 2.075e-004 -3.684 -3.683 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.805e-010 3.516e-010 -9.420 -9.454 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.85 -3.68 -2.84 O2

Initial solution 7. 29/8/2012 13:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.039e-004 4.039e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.608e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.168e-003

Total CO2 (mol/kg) = 4.168e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.01

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551906e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0164 0.8089

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.679e-008 8.936e-008 -7.014 -7.049 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.168e-003

HCO3- 3.585e-003 3.321e-003 -2.445 -2.479 -0.033

CO2 5.232e-004 5.239e-004 -3.281 -3.281 0.001

CaHCO3+ 3.777e-005 3.498e-005 -4.423 -4.456 -0.033

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

CaCO3 2.921e-006 2.925e-006 -5.534 -5.534 0.001

CO3-2 2.853e-006 2.100e-006 -5.545 -5.678 -0.133

MgCO3 6.573e-007 6.581e-007 -6.182 -6.182 0.001

NaHCO3 1.723e-008 1.725e-008 -7.764 -7.763 0.001

NaCO3- 2.679e-010 2.476e-010 -9.572 -9.606 -0.034

Ca 1.332e-003

Ca+2 1.279e-003 9.406e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.777e-005 3.498e-005 -4.423 -4.456 -0.033

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

CaCO3 2.921e-006 2.925e-006 -5.534 -5.534 0.001

CaOH+ 2.677e-009 2.474e-009 -8.572 -8.607 -0.034

CaHSO4+ 4.612e-012 4.263e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 6.065e-026

H2 3.032e-026 3.036e-026 -25.518 -25.518 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

KOH 1.684e-013 1.687e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

MgSO4 5.087e-006 5.094e-006 -5.294 -5.293 0.001

MgCO3 6.573e-007 6.581e-007 -6.182 -6.182 0.001

MgOH+ 1.164e-008 1.076e-008 -7.934 -7.968 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.723e-008 1.725e-008 -7.764 -7.763 0.001

NaSO4- 3.425e-009 3.166e-009 -8.465 -8.500 -0.034

NaCO3- 2.679e-010 2.476e-010 -9.572 -9.606 -0.034

NaOH 9.658e-013 9.671e-013 -12.015 -12.015 0.001

O(0) 4.039e-004

O2 2.019e-004 2.022e-004 -3.695 -3.694 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

MgSO4 5.087e-006 5.094e-006 -5.294 -5.293 0.001

NaSO4- 3.425e-009 3.166e-009 -8.465 -8.500 -0.034

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

HSO4- 4.079e-010 3.770e-010 -9.389 -9.424 -0.034

CaHSO4+ 4.612e-012 4.263e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.38 CO2

Dolomite -0.90 -17.82 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.86 -3.69 -2.84 O2

Initial solution 8. 29/8/2012 13:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.095e-004 4.095e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.160

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.609e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.219e-003

Total CO2 (mol/kg) = 4.219e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.01

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551917e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0579 0.8112

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.828e-008 8.150e-008 -7.054 -7.089 -0.035

H+ 7.428e-008 6.918e-008 -7.129 -7.160 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.219e-003

HCO3- 3.587e-003 3.322e-003 -2.445 -2.479 -0.033

CO2 5.739e-004 5.746e-004 -3.241 -3.241 0.001

CaHCO3+ 3.779e-005 3.500e-005 -4.423 -4.456 -0.033

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

CaCO3 2.665e-006 2.669e-006 -5.574 -5.574 0.001

CO3-2 2.603e-006 1.916e-006 -5.585 -5.718 -0.133

MgCO3 5.997e-007 6.004e-007 -6.222 -6.222 0.001

NaHCO3 1.723e-008 1.725e-008 -7.764 -7.763 0.001

NaCO3- 2.444e-010 2.259e-010 -9.612 -9.646 -0.034

Ca 1.332e-003

Ca+2 1.279e-003 9.408e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.779e-005 3.500e-005 -4.423 -4.456 -0.033

CaSO4 1.254e-005 1.255e-005 -4.902 -4.901 0.001

CaCO3 2.665e-006 2.669e-006 -5.574 -5.574 0.001

CaOH+ 2.442e-009 2.257e-009 -8.612 -8.647 -0.034

CaHSO4+ 5.058e-012 4.675e-012 -11.296 -11.330 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 7.292e-026

H2 3.646e-026 3.651e-026 -25.438 -25.438 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.867 -0.034

KOH 1.536e-013 1.538e-013 -12.814 -12.813 0.001

Mg 5.184e-004

Mg+2 4.977e-004 3.675e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

MgSO4 5.088e-006 5.094e-006 -5.293 -5.293 0.001

MgCO3 5.997e-007 6.004e-007 -6.222 -6.222 0.001

MgOH+ 1.061e-008 9.811e-009 -7.974 -8.008 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.723e-008 1.725e-008 -7.764 -7.763 0.001

NaSO4- 3.425e-009 3.166e-009 -8.465 -8.500 -0.034

NaCO3- 2.444e-010 2.259e-010 -9.612 -9.646 -0.034

NaOH 8.809e-013 8.820e-013 -12.055 -12.055 0.001

O(0) 4.095e-004

O2 2.048e-004 2.050e-004 -3.689 -3.688 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.255e-005 -4.902 -4.901 0.001

MgSO4 5.088e-006 5.094e-006 -5.293 -5.293 0.001

NaSO4- 3.425e-009 3.166e-009 -8.465 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.867 -0.034

HSO4- 4.472e-010 4.133e-010 -9.349 -9.384 -0.034

CaHSO4+ 5.058e-012 4.675e-012 -11.296 -11.330 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.45 -8.74 -8.29 CaCO3

Calcite -0.30 -8.74 -8.44 CaCO3

CO2(g) -1.86 -3.24 -1.38 CO2

Dolomite -0.98 -17.90 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.32 -25.44 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.85 -3.69 -2.84 O2

Initial solution 9. 29/8/2012 13:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.208e-004 4.208e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.157e-003

Total CO2 (mol/kg) = 4.157e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551907e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0096 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.005e-007 9.281e-008 -6.998 -7.032 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.157e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.019e-004 5.025e-004 -3.299 -3.299 0.001

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CO3-2 2.989e-006 2.199e-006 -5.524 -5.658 -0.133

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.537e-026

H2 2.769e-026 2.772e-026 -25.558 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

MgOH+ 1.207e-008 1.115e-008 -7.918 -7.953 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.208e-004

O2 2.104e-004 2.107e-004 -3.677 -3.676 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.886e-010 3.592e-010 -9.410 -9.445 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.68 -2.83 O2

Initial solution 10. 29/8/2012 14:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.026e-004 4.026e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.157e-003

Total CO2 (mol/kg) = 4.157e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0048 0.8079

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.005e-007 9.281e-008 -6.998 -7.032 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.157e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.019e-004 5.025e-004 -3.299 -3.299 0.001

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CO3-2 2.989e-006 2.199e-006 -5.524 -5.658 -0.133

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.537e-026

H2 2.769e-026 2.772e-026 -25.558 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

MgOH+ 1.207e-008 1.115e-008 -7.918 -7.953 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.026e-004

O2 2.013e-004 2.016e-004 -3.696 -3.696 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.886e-010 3.592e-010 -9.410 -9.445 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 11. 29/8/2012 14:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.089e-004 4.089e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551908e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0164 0.8086

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.825e-008 9.069e-008 -7.008 -7.042 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.136e-004 5.143e-004 -3.289 -3.289 0.001

CaHCO3+ 3.789e-005 3.509e-005 -4.421 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 2.993e-006 2.997e-006 -5.524 -5.523 0.001

CO3-2 2.921e-006 2.149e-006 -5.534 -5.668 -0.133

MgCO3 6.715e-007 6.724e-007 -6.173 -6.172 0.001

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaCO3- 2.728e-010 2.521e-010 -9.564 -9.598 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.789e-005 3.509e-005 -4.421 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 2.993e-006 2.997e-006 -5.524 -5.523 0.001

CaOH+ 2.746e-009 2.538e-009 -8.561 -8.596 -0.034

CaHSO4+ 4.509e-012 4.167e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.798e-026

H2 2.899e-026 2.903e-026 -25.538 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.465e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.724e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.715e-007 6.724e-007 -6.173 -6.172 0.001

MgOH+ 1.179e-008 1.090e-008 -7.928 -7.963 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.728e-010 2.521e-010 -9.564 -9.598 -0.034

NaOH 9.883e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 4.089e-004

O2 2.044e-004 2.047e-004 -3.689 -3.689 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.465e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.977e-010 3.675e-010 -9.400 -9.435 -0.034

CaHSO4+ 4.509e-012 4.167e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.38 CO2

Dolomite -0.88 -17.80 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.69 -2.83 O2

Initial solution 12. 29/8/2012 14:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.189e-004 4.189e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.157e-003

Total CO2 (mol/kg) = 4.157e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551907e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0091 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.005e-007 9.281e-008 -6.998 -7.032 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.157e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.019e-004 5.025e-004 -3.299 -3.299 0.001

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CO3-2 2.989e-006 2.199e-006 -5.524 -5.658 -0.133

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.537e-026

H2 2.769e-026 2.772e-026 -25.558 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

MgOH+ 1.207e-008 1.115e-008 -7.918 -7.953 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.189e-004

O2 2.094e-004 2.097e-004 -3.679 -3.678 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.886e-010 3.592e-010 -9.410 -9.445 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.68 -2.83 O2

Initial solution 13. 29/8/2012 14:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.145e-004 4.145e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0279 0.8092

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.601e-008 8.863e-008 -7.018 -7.052 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.596e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.256e-004 5.263e-004 -3.279 -3.279 0.001

CaHCO3+ 3.790e-005 3.510e-005 -4.421 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 2.926e-006 2.929e-006 -5.534 -5.533 0.001

CO3-2 2.855e-006 2.101e-006 -5.544 -5.678 -0.133

MgCO3 6.563e-007 6.572e-007 -6.183 -6.182 0.001

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaCO3- 2.666e-010 2.464e-010 -9.574 -9.608 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.790e-005 3.510e-005 -4.421 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 2.926e-006 2.929e-006 -5.534 -5.533 0.001

CaOH+ 2.684e-009 2.480e-009 -8.571 -8.606 -0.034

CaHSO4+ 4.614e-012 4.264e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.071e-026

H2 3.036e-026 3.040e-026 -25.518 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.465e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.563e-007 6.572e-007 -6.183 -6.182 0.001

MgOH+ 1.153e-008 1.065e-008 -7.938 -7.973 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.666e-010 2.464e-010 -9.574 -9.608 -0.034

NaOH 9.658e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 4.145e-004

O2 2.073e-004 2.075e-004 -3.684 -3.683 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.465e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 4.070e-010 3.761e-010 -9.390 -9.425 -0.034

CaHSO4+ 4.614e-012 4.264e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.38 CO2

Dolomite -0.90 -17.82 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.68 -2.83 O2

Initial solution 14. 29/8/2012 15:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.014e-004 4.014e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.192e-003

Total CO2 (mol/kg) = 4.192e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551913e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0244 0.8090

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.602e-008 8.863e-008 -7.018 -7.052 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.192e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.270e-004 5.277e-004 -3.278 -3.278 0.001

CaHCO3+ 3.809e-005 3.528e-005 -4.419 -4.452 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.941e-006 2.944e-006 -5.532 -5.531 0.001

CO3-2 2.863e-006 2.106e-006 -5.543 -5.676 -0.133

MgCO3 6.579e-007 6.587e-007 -6.182 -6.181 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.673e-010 2.470e-010 -9.573 -9.607 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.453e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.809e-005 3.528e-005 -4.419 -4.452 -0.033

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

CaCO3 2.941e-006 2.944e-006 -5.532 -5.531 0.001

CaOH+ 2.690e-009 2.486e-009 -8.570 -8.604 -0.034

CaHSO4+ 4.623e-012 4.272e-012 -11.335 -11.369 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.071e-026

H2 3.036e-026 3.040e-026 -25.518 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.465e-009 1.354e-009 -8.834 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.066e-006 5.073e-006 -5.295 -5.295 0.001

MgCO3 6.579e-007 6.587e-007 -6.182 -6.181 0.001

MgOH+ 1.152e-008 1.065e-008 -7.938 -7.973 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.420e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.673e-010 2.470e-010 -9.573 -9.607 -0.034

NaOH 9.657e-013 9.669e-013 -12.015 -12.015 0.001

O(0) 4.014e-004

O2 2.007e-004 2.009e-004 -3.697 -3.697 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

MgSO4 5.066e-006 5.073e-006 -5.295 -5.295 0.001

NaSO4- 3.420e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.465e-009 1.354e-009 -8.834 -8.869 -0.034

HSO4- 4.068e-010 3.759e-010 -9.391 -9.425 -0.034

CaHSO4+ 4.623e-012 4.272e-012 -11.335 -11.369 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.38 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 15. 29/8/2012 15:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.982e-004 3.982e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551910e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0223 0.8086

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.159e-004 5.165e-004 -3.287 -3.287 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CO3-2 2.923e-006 2.150e-006 -5.534 -5.668 -0.133

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CaOH+ 2.753e-009 2.544e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 3.982e-004

O2 1.991e-004 1.994e-004 -3.701 -3.700 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.968e-010 3.667e-010 -9.401 -9.436 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.70 -2.83 O2

Initial solution 16. 29/8/2012 15:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.033e-004 4.033e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.160

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.634e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.245e-003

Total CO2 (mol/kg) = 4.245e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551924e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0737 0.8116

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.686e-008 8.017e-008 -7.061 -7.096 -0.035

H+ 7.429e-008 6.918e-008 -7.129 -7.160 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.245e-003

HCO3- 3.607e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.790e-004 5.798e-004 -3.237 -3.237 0.001

CaHCO3+ 3.804e-005 3.523e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.397e-005 -4.821 -4.855 -0.034

CaCO3 2.673e-006 2.677e-006 -5.573 -5.572 0.001

CO3-2 2.606e-006 1.917e-006 -5.584 -5.717 -0.133

MgCO3 5.979e-007 5.987e-007 -6.223 -6.223 0.001

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaCO3- 2.420e-010 2.236e-010 -9.616 -9.650 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.456e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.804e-005 3.523e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.673e-006 2.677e-006 -5.573 -5.572 0.001

CaOH+ 2.454e-009 2.268e-009 -8.610 -8.644 -0.034

CaHSO4+ 5.061e-012 4.677e-012 -11.296 -11.330 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 7.307e-026

H2 3.653e-026 3.658e-026 -25.437 -25.437 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.536e-013 1.538e-013 -12.814 -12.813 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.397e-005 -4.821 -4.855 -0.034

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 5.979e-007 5.987e-007 -6.223 -6.223 0.001

MgOH+ 1.041e-008 9.621e-009 -7.983 -8.017 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

NaCO3- 2.420e-010 2.236e-010 -9.616 -9.650 -0.034

NaOH 8.807e-013 8.819e-013 -12.055 -12.055 0.001

O(0) 4.033e-004

O2 2.016e-004 2.019e-004 -3.695 -3.695 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.452e-010 4.114e-010 -9.351 -9.386 -0.034

CaHSO4+ 5.061e-012 4.677e-012 -11.296 -11.330 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.45 -8.74 -8.29 CaCO3

Calcite -0.30 -8.74 -8.44 CaCO3

CO2(g) -1.86 -3.24 -1.37 CO2

Dolomite -0.98 -17.89 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.32 -25.44 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.69 -2.83 O2

Initial solution 17. 29/8/2012 15:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.939e-004 3.939e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.193e-003

Total CO2 (mol/kg) = 4.193e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551912e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0311 0.8091

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.193e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.279e-004 5.286e-004 -3.277 -3.277 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CO3-2 2.856e-006 2.101e-006 -5.544 -5.678 -0.133

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CaOH+ 2.691e-009 2.486e-009 -8.570 -8.604 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

MgOH+ 1.141e-008 1.055e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

NaOH 9.657e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 3.939e-004

O2 1.969e-004 1.972e-004 -3.706 -3.705 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.061e-010 3.752e-010 -9.391 -9.426 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.71 -2.83 O2

Initial solution 18. 29/8/2012 16:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.882e-004 3.882e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.193e-003

Total CO2 (mol/kg) = 4.193e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551912e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0295 0.8091

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.193e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.279e-004 5.286e-004 -3.277 -3.277 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CO3-2 2.856e-006 2.101e-006 -5.544 -5.678 -0.133

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CaOH+ 2.691e-009 2.486e-009 -8.570 -8.604 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

MgOH+ 1.141e-008 1.055e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

NaOH 9.657e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 3.882e-004

O2 1.941e-004 1.944e-004 -3.712 -3.711 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.061e-010 3.752e-010 -9.391 -9.426 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 19. 29/8/2012 16:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.876e-004 3.876e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.160

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.634e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.245e-003

Total CO2 (mol/kg) = 4.245e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551922e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0694 0.8114

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.686e-008 8.017e-008 -7.061 -7.096 -0.035

H+ 7.429e-008 6.918e-008 -7.129 -7.160 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.245e-003

HCO3- 3.607e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.790e-004 5.798e-004 -3.237 -3.237 0.001

CaHCO3+ 3.804e-005 3.523e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.397e-005 -4.821 -4.855 -0.034

CaCO3 2.673e-006 2.677e-006 -5.573 -5.572 0.001

CO3-2 2.606e-006 1.917e-006 -5.584 -5.717 -0.133

MgCO3 5.979e-007 5.987e-007 -6.223 -6.223 0.001

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaCO3- 2.420e-010 2.236e-010 -9.616 -9.650 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.456e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.804e-005 3.523e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.673e-006 2.677e-006 -5.573 -5.572 0.001

CaOH+ 2.454e-009 2.268e-009 -8.610 -8.644 -0.034

CaHSO4+ 5.061e-012 4.677e-012 -11.296 -11.330 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 7.307e-026

H2 3.653e-026 3.658e-026 -25.437 -25.437 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.536e-013 1.538e-013 -12.814 -12.813 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.397e-005 -4.821 -4.855 -0.034

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 5.979e-007 5.987e-007 -6.223 -6.223 0.001

MgOH+ 1.041e-008 9.621e-009 -7.983 -8.017 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

NaCO3- 2.420e-010 2.236e-010 -9.616 -9.650 -0.034

NaOH 8.807e-013 8.819e-013 -12.055 -12.055 0.001

O(0) 3.876e-004

O2 1.938e-004 1.941e-004 -3.713 -3.712 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.452e-010 4.114e-010 -9.351 -9.386 -0.034

CaHSO4+ 5.061e-012 4.677e-012 -11.296 -11.330 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.45 -8.74 -8.29 CaCO3

Calcite -0.30 -8.74 -8.44 CaCO3

CO2(g) -1.86 -3.24 -1.37 CO2

Dolomite -0.98 -17.89 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.32 -25.44 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 20. 29/8/2012 16:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.682e-003 3.682e-003

Ca 1.343e-003 1.343e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.751e-004 3.751e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.645e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.205e-003

Total CO2 (mol/kg) = 4.205e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.335e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.11

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551914e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0258 0.8088

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.776e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.205e-003

HCO3- 3.616e-003 3.348e-003 -2.442 -2.475 -0.033

CO2 5.293e-004 5.300e-004 -3.276 -3.276 0.001

CaHCO3+ 3.822e-005 3.539e-005 -4.418 -4.451 -0.033

MgHCO3+ 1.514e-005 1.399e-005 -4.820 -4.854 -0.034

CaCO3 2.945e-006 2.949e-006 -5.531 -5.530 0.001

CO3-2 2.865e-006 2.107e-006 -5.543 -5.676 -0.133

MgCO3 6.569e-007 6.577e-007 -6.183 -6.182 0.001

NaHCO3 1.737e-008 1.739e-008 -7.760 -7.760 0.001

NaCO3- 2.660e-010 2.458e-010 -9.575 -9.609 -0.034

Ca 1.343e-003

Ca+2 1.289e-003 9.477e-004 -2.890 -3.023 -0.134

CaHCO3+ 3.822e-005 3.539e-005 -4.418 -4.451 -0.033

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

CaCO3 2.945e-006 2.949e-006 -5.531 -5.530 0.001

CaOH+ 2.697e-009 2.493e-009 -8.569 -8.603 -0.034

CaHSO4+ 4.625e-012 4.273e-012 -11.335 -11.369 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.671e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.514e-005 1.399e-005 -4.820 -4.854 -0.034

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

MgCO3 6.569e-007 6.577e-007 -6.183 -6.182 0.001

MgOH+ 1.141e-008 1.054e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.986e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.737e-008 1.739e-008 -7.760 -7.760 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.660e-010 2.458e-010 -9.575 -9.609 -0.034

NaOH 9.656e-013 9.669e-013 -12.015 -12.015 0.001

O(0) 3.751e-004

O2 1.876e-004 1.878e-004 -3.727 -3.726 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.164e-005 -4.010 -4.145 -0.135

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.059e-010 3.751e-010 -9.392 -9.426 -0.034

CaHSO4+ 4.625e-012 4.273e-012 -11.335 -11.369 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.73 -2.83 O2

Initial solution 21. 29/8/2012 16:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.682e-003 3.682e-003

Ca 1.343e-003 1.343e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.776e-004 3.776e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.190

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.645e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.217e-003

Total CO2 (mol/kg) = 4.217e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.335e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.11

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551917e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0365 0.8095

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.307e-008 8.591e-008 -7.031 -7.066 -0.035

H+ 6.934e-008 6.457e-008 -7.159 -7.190 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.217e-003

HCO3- 3.616e-003 3.349e-003 -2.442 -2.475 -0.033

CO2 5.417e-004 5.424e-004 -3.266 -3.266 0.001

CaHCO3+ 3.822e-005 3.540e-005 -4.418 -4.451 -0.033

MgHCO3+ 1.515e-005 1.400e-005 -4.820 -4.854 -0.034

CaCO3 2.878e-006 2.882e-006 -5.541 -5.540 0.001

CO3-2 2.800e-006 2.059e-006 -5.553 -5.686 -0.133

MgCO3 6.420e-007 6.428e-007 -6.192 -6.192 0.001

NaHCO3 1.737e-008 1.739e-008 -7.760 -7.760 0.001

NaCO3- 2.599e-010 2.402e-010 -9.585 -9.619 -0.034

Ca 1.343e-003

Ca+2 1.290e-003 9.478e-004 -2.890 -3.023 -0.134

CaHCO3+ 3.822e-005 3.540e-005 -4.418 -4.451 -0.033

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

CaCO3 2.878e-006 2.882e-006 -5.541 -5.540 0.001

CaOH+ 2.636e-009 2.436e-009 -8.579 -8.613 -0.034

CaHSO4+ 4.733e-012 4.373e-012 -11.325 -11.359 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.364e-026

H2 3.182e-026 3.186e-026 -25.497 -25.497 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.646e-013 1.648e-013 -12.784 -12.783 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.671e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.515e-005 1.400e-005 -4.820 -4.854 -0.034

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

MgCO3 6.420e-007 6.428e-007 -6.192 -6.192 0.001

MgOH+ 1.115e-008 1.030e-008 -7.953 -7.987 -0.034

Na 1.001e-005

Na+ 9.986e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.737e-008 1.739e-008 -7.760 -7.760 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.599e-010 2.402e-010 -9.585 -9.619 -0.034

NaOH 9.436e-013 9.449e-013 -12.025 -12.025 0.001

O(0) 3.776e-004

O2 1.888e-004 1.891e-004 -3.724 -3.723 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.164e-005 -4.010 -4.145 -0.135

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.153e-010 3.838e-010 -9.382 -9.416 -0.034

CaHSO4+ 4.733e-012 4.373e-012 -11.325 -11.359 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.42 -8.71 -8.29 CaCO3

Calcite -0.27 -8.71 -8.44 CaCO3

CO2(g) -1.89 -3.27 -1.37 CO2

Dolomite -0.92 -17.83 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.38 -25.50 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 22. 29/8/2012 17:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.682e-003 3.682e-003

Ca 1.343e-003 1.343e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.695e-004 3.695e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.645e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.193e-003

Total CO2 (mol/kg) = 4.193e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.335e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.11

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0142 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.746e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.193e-003

HCO3- 3.615e-003 3.348e-003 -2.442 -2.475 -0.033

CO2 5.173e-004 5.179e-004 -3.286 -3.286 0.001

CaHCO3+ 3.821e-005 3.539e-005 -4.418 -4.451 -0.033

MgHCO3+ 1.514e-005 1.399e-005 -4.820 -4.854 -0.034

CaCO3 3.013e-006 3.017e-006 -5.521 -5.520 0.001

CO3-2 2.931e-006 2.156e-006 -5.533 -5.666 -0.133

MgCO3 6.721e-007 6.730e-007 -6.173 -6.172 0.001

NaHCO3 1.736e-008 1.739e-008 -7.760 -7.760 0.001

NaCO3- 2.721e-010 2.515e-010 -9.565 -9.600 -0.034

Ca 1.343e-003

Ca+2 1.289e-003 9.477e-004 -2.890 -3.023 -0.134

CaHCO3+ 3.821e-005 3.539e-005 -4.418 -4.451 -0.033

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

CaCO3 3.013e-006 3.017e-006 -5.521 -5.520 0.001

CaOH+ 2.760e-009 2.550e-009 -8.559 -8.593 -0.034

CaHSO4+ 4.519e-012 4.176e-012 -11.345 -11.379 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.671e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.514e-005 1.399e-005 -4.820 -4.854 -0.034

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

MgCO3 6.721e-007 6.730e-007 -6.173 -6.172 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.986e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.736e-008 1.739e-008 -7.760 -7.760 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.721e-010 2.515e-010 -9.565 -9.600 -0.034

NaOH 9.881e-013 9.894e-013 -12.005 -12.005 0.001

O(0) 3.695e-004

O2 1.847e-004 1.850e-004 -3.733 -3.733 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.164e-005 -4.010 -4.145 -0.135

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.966e-010 3.665e-010 -9.402 -9.436 -0.034

CaHSO4+ 4.519e-012 4.176e-012 -11.345 -11.379 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.90 -3.73 -2.83 O2

Initial solution 23. 29/8/2012 17:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.807e-004 3.807e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551906e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0074 0.8078

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.807e-004

O2 1.904e-004 1.906e-004 -3.720 -3.720 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 24. 29/8/2012 17:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.682e-003 3.682e-003

Ca 1.343e-003 1.343e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.007e-004 4.007e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.645e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.205e-003

Total CO2 (mol/kg) = 4.205e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.335e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.11

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551916e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0330 0.8093

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.776e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.205e-003

HCO3- 3.616e-003 3.348e-003 -2.442 -2.475 -0.033

CO2 5.293e-004 5.300e-004 -3.276 -3.276 0.001

CaHCO3+ 3.822e-005 3.539e-005 -4.418 -4.451 -0.033

MgHCO3+ 1.514e-005 1.399e-005 -4.820 -4.854 -0.034

CaCO3 2.945e-006 2.949e-006 -5.531 -5.530 0.001

CO3-2 2.865e-006 2.107e-006 -5.543 -5.676 -0.133

MgCO3 6.569e-007 6.577e-007 -6.183 -6.182 0.001

NaHCO3 1.737e-008 1.739e-008 -7.760 -7.760 0.001

NaCO3- 2.660e-010 2.458e-010 -9.575 -9.609 -0.034

Ca 1.343e-003

Ca+2 1.289e-003 9.477e-004 -2.890 -3.023 -0.134

CaHCO3+ 3.822e-005 3.539e-005 -4.418 -4.451 -0.033

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

CaCO3 2.945e-006 2.949e-006 -5.531 -5.530 0.001

CaOH+ 2.697e-009 2.493e-009 -8.569 -8.603 -0.034

CaHSO4+ 4.625e-012 4.273e-012 -11.335 -11.369 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.671e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.514e-005 1.399e-005 -4.820 -4.854 -0.034

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

MgCO3 6.569e-007 6.577e-007 -6.183 -6.182 0.001

MgOH+ 1.141e-008 1.054e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.986e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.737e-008 1.739e-008 -7.760 -7.760 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.660e-010 2.458e-010 -9.575 -9.609 -0.034

NaOH 9.656e-013 9.669e-013 -12.015 -12.015 0.001

O(0) 4.007e-004

O2 2.004e-004 2.006e-004 -3.698 -3.698 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.164e-005 -4.010 -4.145 -0.135

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.059e-010 3.751e-010 -9.392 -9.426 -0.034

CaHSO4+ 4.625e-012 4.273e-012 -11.335 -11.369 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 25. 29/8/2012 17:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.826e-004 3.826e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551906e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0080 0.8078

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.826e-004

O2 1.913e-004 1.916e-004 -3.718 -3.718 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.72 -2.83 O2

Initial solution 26. 29/8/2012 18:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.901e-004 3.901e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551910e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0201 0.8085

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.159e-004 5.165e-004 -3.287 -3.287 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CO3-2 2.923e-006 2.150e-006 -5.534 -5.668 -0.133

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CaOH+ 2.753e-009 2.544e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 3.901e-004

O2 1.951e-004 1.953e-004 -3.710 -3.709 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.968e-010 3.667e-010 -9.401 -9.436 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 27. 29/8/2012 18:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.814e-004 3.814e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.193e-003

Total CO2 (mol/kg) = 4.193e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0276 0.8089

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.193e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.279e-004 5.286e-004 -3.277 -3.277 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CO3-2 2.856e-006 2.101e-006 -5.544 -5.678 -0.133

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CaOH+ 2.691e-009 2.486e-009 -8.570 -8.604 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

MgOH+ 1.141e-008 1.055e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

NaOH 9.657e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 3.814e-004

O2 1.907e-004 1.909e-004 -3.720 -3.719 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.061e-010 3.752e-010 -9.391 -9.426 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 28. 29/8/2012 18:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.751e-004 3.751e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.190

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.206e-003

Total CO2 (mol/kg) = 4.206e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551913e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0358 0.8094

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.307e-008 8.591e-008 -7.031 -7.066 -0.035

H+ 6.933e-008 6.457e-008 -7.159 -7.190 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.206e-003

HCO3- 3.606e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.403e-004 5.410e-004 -3.267 -3.267 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CO3-2 2.792e-006 2.054e-006 -5.554 -5.687 -0.133

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CaOH+ 2.630e-009 2.430e-009 -8.580 -8.614 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.364e-026

H2 3.182e-026 3.186e-026 -25.497 -25.497 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.646e-013 1.648e-013 -12.784 -12.783 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

MgOH+ 1.115e-008 1.031e-008 -7.953 -7.987 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

NaOH 9.437e-013 9.449e-013 -12.025 -12.025 0.001

O(0) 3.751e-004

O2 1.876e-004 1.878e-004 -3.727 -3.726 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.155e-010 3.840e-010 -9.381 -9.416 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.42 -8.71 -8.29 CaCO3

Calcite -0.27 -8.71 -8.44 CaCO3

CO2(g) -1.89 -3.27 -1.37 CO2

Dolomite -0.92 -17.83 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.38 -25.50 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.73 -2.83 O2

Initial solution 29. 29/8/2012 18:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.682e-003 3.682e-003

Ca 1.343e-003 1.343e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.870e-004 3.870e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.645e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.205e-003

Total CO2 (mol/kg) = 4.205e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.335e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.11

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551915e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0292 0.8090

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.776e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.205e-003

HCO3- 3.616e-003 3.348e-003 -2.442 -2.475 -0.033

CO2 5.293e-004 5.300e-004 -3.276 -3.276 0.001

CaHCO3+ 3.822e-005 3.539e-005 -4.418 -4.451 -0.033

MgHCO3+ 1.514e-005 1.399e-005 -4.820 -4.854 -0.034

CaCO3 2.945e-006 2.949e-006 -5.531 -5.530 0.001

CO3-2 2.865e-006 2.107e-006 -5.543 -5.676 -0.133

MgCO3 6.569e-007 6.577e-007 -6.183 -6.182 0.001

NaHCO3 1.737e-008 1.739e-008 -7.760 -7.760 0.001

NaCO3- 2.660e-010 2.458e-010 -9.575 -9.609 -0.034

Ca 1.343e-003

Ca+2 1.289e-003 9.477e-004 -2.890 -3.023 -0.134

CaHCO3+ 3.822e-005 3.539e-005 -4.418 -4.451 -0.033

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

CaCO3 2.945e-006 2.949e-006 -5.531 -5.530 0.001

CaOH+ 2.697e-009 2.493e-009 -8.569 -8.603 -0.034

CaHSO4+ 4.625e-012 4.273e-012 -11.335 -11.369 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.671e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.514e-005 1.399e-005 -4.820 -4.854 -0.034

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

MgCO3 6.569e-007 6.577e-007 -6.183 -6.182 0.001

MgOH+ 1.141e-008 1.054e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.986e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.737e-008 1.739e-008 -7.760 -7.760 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.660e-010 2.458e-010 -9.575 -9.609 -0.034

NaOH 9.656e-013 9.669e-013 -12.015 -12.015 0.001

O(0) 3.870e-004

O2 1.935e-004 1.937e-004 -3.713 -3.713 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.164e-005 -4.010 -4.145 -0.135

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.059e-010 3.751e-010 -9.392 -9.426 -0.034

CaHSO4+ 4.625e-012 4.273e-012 -11.335 -11.369 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 30. 29/8/2012 19:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.964e-004 3.964e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551908e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0118 0.8080

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.964e-004

O2 1.982e-004 1.984e-004 -3.703 -3.702 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.70 -2.83 O2

Initial solution 31. 29/8/2012 19:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.826e-004 3.826e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.193e-003

Total CO2 (mol/kg) = 4.193e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0280 0.8090

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.193e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.279e-004 5.286e-004 -3.277 -3.277 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CO3-2 2.856e-006 2.101e-006 -5.544 -5.678 -0.133

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CaOH+ 2.691e-009 2.486e-009 -8.570 -8.604 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

MgOH+ 1.141e-008 1.055e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

NaOH 9.657e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 3.826e-004

O2 1.913e-004 1.916e-004 -3.718 -3.718 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.061e-010 3.752e-010 -9.391 -9.426 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.72 -2.83 O2

Initial solution 32. 29/8/2012 19:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.895e-004 3.895e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.110

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.635e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.317e-003

Total CO2 (mol/kg) = 4.317e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551937e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.1199 0.8143

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

H+ 8.335e-008 7.762e-008 -7.079 -7.110 -0.031

OH- 7.741e-008 7.145e-008 -7.111 -7.146 -0.035

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.317e-003

HCO3- 3.608e-003 3.342e-003 -2.443 -2.476 -0.033

CO2 6.499e-004 6.508e-004 -3.187 -3.187 0.001

CaHCO3+ 3.806e-005 3.525e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.512e-005 1.397e-005 -4.820 -4.855 -0.034

CaCO3 2.384e-006 2.387e-006 -5.623 -5.622 0.001

CO3-2 2.323e-006 1.709e-006 -5.634 -5.767 -0.133

MgCO3 5.331e-007 5.338e-007 -6.273 -6.273 0.001

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaCO3- 2.158e-010 1.994e-010 -9.666 -9.700 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.458e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.806e-005 3.525e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

CaCO3 2.384e-006 2.387e-006 -5.623 -5.622 0.001

CaOH+ 2.188e-009 2.022e-009 -8.660 -8.694 -0.034

CaHSO4+ 5.680e-012 5.249e-012 -11.246 -11.280 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 9.199e-026

H2 4.599e-026 4.605e-026 -25.337 -25.337 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.369e-013 1.371e-013 -12.864 -12.863 0.001

Mg 5.184e-004

Mg+2 4.977e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.512e-005 1.397e-005 -4.820 -4.855 -0.034

MgSO4 5.055e-006 5.062e-006 -5.296 -5.296 0.001

MgCO3 5.331e-007 5.338e-007 -6.273 -6.273 0.001

MgOH+ 9.280e-009 8.575e-009 -8.032 -8.067 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

NaCO3- 2.158e-010 1.994e-010 -9.666 -9.700 -0.034

NaOH 7.849e-013 7.860e-013 -12.105 -12.105 0.001

O(0) 3.895e-004

O2 1.947e-004 1.950e-004 -3.711 -3.710 0.001

S(6) 1.154e-004

SO4-2 9.774e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

MgSO4 5.055e-006 5.062e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.995e-010 4.616e-010 -9.301 -9.336 -0.034

CaHSO4+ 5.680e-012 5.249e-012 -11.246 -11.280 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.50 -8.79 -8.29 CaCO3

Calcite -0.35 -8.79 -8.44 CaCO3

CO2(g) -1.81 -3.19 -1.37 CO2

Dolomite -1.08 -17.99 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.22 -25.34 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 33. 29/8/2012 19:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.189e-004 4.189e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.190

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.206e-003

Total CO2 (mol/kg) = 4.206e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551917e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0478 0.8101

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.307e-008 8.591e-008 -7.031 -7.066 -0.035

H+ 6.933e-008 6.457e-008 -7.159 -7.190 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.206e-003

HCO3- 3.606e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.403e-004 5.410e-004 -3.267 -3.267 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CO3-2 2.792e-006 2.054e-006 -5.554 -5.687 -0.133

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CaOH+ 2.630e-009 2.430e-009 -8.580 -8.614 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.364e-026

H2 3.182e-026 3.186e-026 -25.497 -25.497 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.646e-013 1.648e-013 -12.784 -12.783 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

MgOH+ 1.115e-008 1.031e-008 -7.953 -7.987 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

NaOH 9.437e-013 9.449e-013 -12.025 -12.025 0.001

O(0) 4.189e-004

O2 2.094e-004 2.097e-004 -3.679 -3.678 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.155e-010 3.840e-010 -9.381 -9.416 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.42 -8.71 -8.29 CaCO3

Calcite -0.27 -8.71 -8.44 CaCO3

CO2(g) -1.89 -3.27 -1.37 CO2

Dolomite -0.92 -17.83 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.38 -25.50 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.68 -2.83 O2

Initial solution 34. 29/8/2012 20:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.801e-004 3.801e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551909e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0172 0.8083

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.159e-004 5.165e-004 -3.287 -3.287 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CO3-2 2.923e-006 2.150e-006 -5.534 -5.668 -0.133

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CaOH+ 2.753e-009 2.544e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 3.801e-004

O2 1.901e-004 1.903e-004 -3.721 -3.721 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.968e-010 3.667e-010 -9.401 -9.436 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 35. 29/8/2012 20:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.114e-004 4.114e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.193e-003

Total CO2 (mol/kg) = 4.193e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551914e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0358 0.8094

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.193e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.279e-004 5.286e-004 -3.277 -3.277 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CO3-2 2.856e-006 2.101e-006 -5.544 -5.678 -0.133

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CaOH+ 2.691e-009 2.486e-009 -8.570 -8.604 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

MgOH+ 1.141e-008 1.055e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

NaOH 9.657e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 4.114e-004

O2 2.057e-004 2.060e-004 -3.687 -3.686 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.061e-010 3.752e-010 -9.391 -9.426 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.69 -2.83 O2

Initial solution 36. 29/8/2012 20:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.851e-004 3.851e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.190

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.206e-003

Total CO2 (mol/kg) = 4.206e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551914e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0387 0.8096

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.307e-008 8.591e-008 -7.031 -7.066 -0.035

H+ 6.933e-008 6.457e-008 -7.159 -7.190 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.206e-003

HCO3- 3.606e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.403e-004 5.410e-004 -3.267 -3.267 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CO3-2 2.792e-006 2.054e-006 -5.554 -5.687 -0.133

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CaOH+ 2.630e-009 2.430e-009 -8.580 -8.614 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.364e-026

H2 3.182e-026 3.186e-026 -25.497 -25.497 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.646e-013 1.648e-013 -12.784 -12.783 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

MgOH+ 1.115e-008 1.031e-008 -7.953 -7.987 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

NaOH 9.437e-013 9.449e-013 -12.025 -12.025 0.001

O(0) 3.851e-004

O2 1.926e-004 1.928e-004 -3.715 -3.715 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.155e-010 3.840e-010 -9.381 -9.416 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.42 -8.71 -8.29 CaCO3

Calcite -0.27 -8.71 -8.44 CaCO3

CO2(g) -1.89 -3.27 -1.37 CO2

Dolomite -0.92 -17.83 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.38 -25.50 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 37. 29/8/2012 20:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.907e-004 3.907e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.190

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.206e-003

Total CO2 (mol/kg) = 4.206e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551915e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0402 0.8097

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.307e-008 8.591e-008 -7.031 -7.066 -0.035

H+ 6.933e-008 6.457e-008 -7.159 -7.190 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.206e-003

HCO3- 3.606e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.403e-004 5.410e-004 -3.267 -3.267 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CO3-2 2.792e-006 2.054e-006 -5.554 -5.687 -0.133

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CaOH+ 2.630e-009 2.430e-009 -8.580 -8.614 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.364e-026

H2 3.182e-026 3.186e-026 -25.497 -25.497 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.646e-013 1.648e-013 -12.784 -12.783 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

MgOH+ 1.115e-008 1.031e-008 -7.953 -7.987 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

NaOH 9.437e-013 9.449e-013 -12.025 -12.025 0.001

O(0) 3.907e-004

O2 1.954e-004 1.956e-004 -3.709 -3.709 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.155e-010 3.840e-010 -9.381 -9.416 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.42 -8.71 -8.29 CaCO3

Calcite -0.27 -8.71 -8.44 CaCO3

CO2(g) -1.89 -3.27 -1.37 CO2

Dolomite -0.92 -17.83 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.38 -25.50 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.71 -2.83 O2

Initial solution 38. 29/8/2012 21:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.001e-004 4.001e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.190

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.206e-003

Total CO2 (mol/kg) = 4.206e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551916e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0428 0.8098

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.307e-008 8.591e-008 -7.031 -7.066 -0.035

H+ 6.933e-008 6.457e-008 -7.159 -7.190 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.206e-003

HCO3- 3.606e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.403e-004 5.410e-004 -3.267 -3.267 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CO3-2 2.792e-006 2.054e-006 -5.554 -5.687 -0.133

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CaOH+ 2.630e-009 2.430e-009 -8.580 -8.614 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.364e-026

H2 3.182e-026 3.186e-026 -25.497 -25.497 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.646e-013 1.648e-013 -12.784 -12.783 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

MgOH+ 1.115e-008 1.031e-008 -7.953 -7.987 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

NaOH 9.437e-013 9.449e-013 -12.025 -12.025 0.001

O(0) 4.001e-004

O2 2.001e-004 2.003e-004 -3.699 -3.698 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.155e-010 3.840e-010 -9.381 -9.416 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.42 -8.71 -8.29 CaCO3

Calcite -0.27 -8.71 -8.44 CaCO3

CO2(g) -1.89 -3.27 -1.37 CO2

Dolomite -0.92 -17.83 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.38 -25.50 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 39. 29/8/2012 21:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.170e-004 4.170e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.270

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.632e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.113e-003

Total CO2 (mol/kg) = 4.113e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551899e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9673 0.8055

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.119e-007 1.033e-007 -6.951 -6.986 -0.035

H+ 5.767e-008 5.370e-008 -7.239 -7.270 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.113e-003

HCO3- 3.604e-003 3.337e-003 -2.443 -2.477 -0.033

CO2 4.491e-004 4.497e-004 -3.348 -3.347 0.001

CaHCO3+ 3.799e-005 3.518e-005 -4.420 -4.454 -0.033

MgHCO3+ 1.510e-005 1.395e-005 -4.821 -4.855 -0.034

CaCO3 3.439e-006 3.444e-006 -5.464 -5.463 0.001

CO3-2 3.354e-006 2.467e-006 -5.474 -5.608 -0.133

MgCO3 7.694e-007 7.704e-007 -6.114 -6.113 0.001

NaHCO3 1.731e-008 1.733e-008 -7.762 -7.761 0.001

NaCO3- 3.115e-010 2.878e-010 -9.507 -9.541 -0.034

Ca 1.339e-003

Ca+2 1.285e-003 9.451e-004 -2.891 -3.025 -0.134

CaHCO3+ 3.799e-005 3.518e-005 -4.420 -4.454 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.439e-006 3.444e-006 -5.464 -5.463 0.001

CaOH+ 3.160e-009 2.920e-009 -8.500 -8.535 -0.034

CaHSO4+ 3.927e-012 3.629e-012 -11.406 -11.440 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 4.403e-026

H2 2.201e-026 2.204e-026 -25.657 -25.657 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.979e-013 1.981e-013 -12.704 -12.703 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.395e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.060e-006 -5.296 -5.296 0.001

MgCO3 7.694e-007 7.704e-007 -6.114 -6.113 0.001

MgOH+ 1.341e-008 1.239e-008 -7.873 -7.907 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.731e-008 1.733e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 3.115e-010 2.878e-010 -9.507 -9.541 -0.034

NaOH 1.135e-012 1.136e-012 -11.945 -11.945 0.001

O(0) 4.170e-004

O2 2.085e-004 2.088e-004 -3.681 -3.680 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.060e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.456e-010 3.194e-010 -9.461 -9.496 -0.034

CaHSO4+ 3.927e-012 3.629e-012 -11.406 -11.440 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.34 -8.63 -8.29 CaCO3

Calcite -0.19 -8.63 -8.44 CaCO3

CO2(g) -1.97 -3.35 -1.37 CO2

Dolomite -0.76 -17.68 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.54 -25.66 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.68 -2.83 O2

Initial solution 40. 29/8/2012 21:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.789e-004 3.789e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.190

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.206e-003

Total CO2 (mol/kg) = 4.206e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551913e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0369 0.8095

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.307e-008 8.591e-008 -7.031 -7.066 -0.035

H+ 6.933e-008 6.457e-008 -7.159 -7.190 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.206e-003

HCO3- 3.606e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.403e-004 5.410e-004 -3.267 -3.267 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CO3-2 2.792e-006 2.054e-006 -5.554 -5.687 -0.133

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CaOH+ 2.630e-009 2.430e-009 -8.580 -8.614 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.364e-026

H2 3.182e-026 3.186e-026 -25.497 -25.497 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.646e-013 1.648e-013 -12.784 -12.783 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

MgOH+ 1.115e-008 1.031e-008 -7.953 -7.987 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

NaOH 9.437e-013 9.449e-013 -12.025 -12.025 0.001

O(0) 3.789e-004

O2 1.894e-004 1.897e-004 -3.723 -3.722 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.155e-010 3.840e-010 -9.381 -9.416 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.42 -8.71 -8.29 CaCO3

Calcite -0.27 -8.71 -8.44 CaCO3

CO2(g) -1.89 -3.27 -1.37 CO2

Dolomite -0.92 -17.83 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.38 -25.50 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 41. 29/8/2012 21:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.757e-004 3.757e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.160

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.634e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.245e-003

Total CO2 (mol/kg) = 4.245e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551921e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0660 0.8112

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.686e-008 8.017e-008 -7.061 -7.096 -0.035

H+ 7.429e-008 6.918e-008 -7.129 -7.160 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.245e-003

HCO3- 3.607e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.790e-004 5.798e-004 -3.237 -3.237 0.001

CaHCO3+ 3.804e-005 3.523e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.397e-005 -4.821 -4.855 -0.034

CaCO3 2.673e-006 2.677e-006 -5.573 -5.572 0.001

CO3-2 2.606e-006 1.917e-006 -5.584 -5.717 -0.133

MgCO3 5.979e-007 5.987e-007 -6.223 -6.223 0.001

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaCO3- 2.420e-010 2.236e-010 -9.616 -9.650 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.456e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.804e-005 3.523e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.673e-006 2.677e-006 -5.573 -5.572 0.001

CaOH+ 2.454e-009 2.268e-009 -8.610 -8.644 -0.034

CaHSO4+ 5.061e-012 4.677e-012 -11.296 -11.330 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 7.307e-026

H2 3.653e-026 3.658e-026 -25.437 -25.437 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.536e-013 1.538e-013 -12.814 -12.813 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.397e-005 -4.821 -4.855 -0.034

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 5.979e-007 5.987e-007 -6.223 -6.223 0.001

MgOH+ 1.041e-008 9.621e-009 -7.983 -8.017 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

NaCO3- 2.420e-010 2.236e-010 -9.616 -9.650 -0.034

NaOH 8.807e-013 8.819e-013 -12.055 -12.055 0.001

O(0) 3.757e-004

O2 1.879e-004 1.881e-004 -3.726 -3.726 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.452e-010 4.114e-010 -9.351 -9.386 -0.034

CaHSO4+ 5.061e-012 4.677e-012 -11.296 -11.330 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.45 -8.74 -8.29 CaCO3

Calcite -0.30 -8.74 -8.44 CaCO3

CO2(g) -1.86 -3.24 -1.37 CO2

Dolomite -0.98 -17.89 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.32 -25.44 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.73 -2.83 O2

Initial solution 42. 29/8/2012 22:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.745e-004 3.745e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.193e-003

Total CO2 (mol/kg) = 4.193e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0256 0.8088

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.193e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.279e-004 5.286e-004 -3.277 -3.277 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CO3-2 2.856e-006 2.101e-006 -5.544 -5.678 -0.133

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CaOH+ 2.691e-009 2.486e-009 -8.570 -8.604 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

MgOH+ 1.141e-008 1.055e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

NaOH 9.657e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 3.745e-004

O2 1.872e-004 1.875e-004 -3.728 -3.727 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.061e-010 3.752e-010 -9.391 -9.426 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.73 -2.83 O2

Initial solution 43. 29/8/2012 22:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.045e-004 4.045e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99896

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.147e-003

Total CO2 (mol/kg) = 4.147e-003

Temperature (deg C) = 17.400

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0027 0.8072

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.036e-007 9.560e-008 -6.985 -7.020 -0.035

H+ 6.179e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.147e-003

HCO3- 3.605e-003 3.338e-003 -2.443 -2.476 -0.033

CO2 4.822e-004 4.828e-004 -3.317 -3.316 0.001

CaHCO3+ 3.793e-005 3.513e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.510e-005 1.395e-005 -4.821 -4.855 -0.034

CaCO3 3.199e-006 3.203e-006 -5.495 -5.494 0.001

CO3-2 3.123e-006 2.298e-006 -5.505 -5.639 -0.133

MgCO3 7.155e-007 7.164e-007 -6.145 -6.145 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.885e-010 2.666e-010 -9.540 -9.574 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.793e-005 3.513e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.199e-006 3.203e-006 -5.495 -5.494 0.001

CaOH+ 2.950e-009 2.726e-009 -8.530 -8.564 -0.034

CaHSO4+ 4.202e-012 3.883e-012 -11.377 -11.411 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.060e-026

H2 2.530e-026 2.534e-026 -25.597 -25.596 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.395e-005 -4.821 -4.855 -0.034

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

MgCO3 7.155e-007 7.164e-007 -6.145 -6.145 0.001

MgOH+ 1.240e-008 1.146e-008 -7.907 -7.941 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.885e-010 2.666e-010 -9.540 -9.574 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 4.045e-004

O2 2.023e-004 2.025e-004 -3.694 -3.694 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

HSO4- 3.697e-010 3.416e-010 -9.432 -9.466 -0.034

CaHSO4+ 4.202e-012 3.883e-012 -11.377 -11.411 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.37 CO2

Dolomite -0.83 -17.74 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.69 -2.83 O2

Initial solution 44. 29/8/2012 22:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.801e-004 3.801e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.130

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.634e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.287e-003

Total CO2 (mol/kg) = 4.287e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551930e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0972 0.8130

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.106e-008 7.482e-008 -7.091 -7.126 -0.035

H+ 7.960e-008 7.413e-008 -7.099 -7.130 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.287e-003

HCO3- 3.608e-003 3.341e-003 -2.443 -2.476 -0.033

CO2 6.206e-004 6.214e-004 -3.207 -3.207 0.001

CaHCO3+ 3.805e-005 3.524e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.512e-005 1.397e-005 -4.821 -4.855 -0.034

CaCO3 2.496e-006 2.499e-006 -5.603 -5.602 0.001

CO3-2 2.433e-006 1.789e-006 -5.614 -5.747 -0.133

MgCO3 5.582e-007 5.589e-007 -6.253 -6.253 0.001

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaCO3- 2.259e-010 2.087e-010 -9.646 -9.680 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.457e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.805e-005 3.524e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

CaCO3 2.496e-006 2.499e-006 -5.603 -5.602 0.001

CaOH+ 2.291e-009 2.117e-009 -8.640 -8.674 -0.034

CaHSO4+ 5.424e-012 5.012e-012 -11.266 -11.300 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 8.390e-026

H2 4.195e-026 4.200e-026 -25.377 -25.377 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.433e-013 1.435e-013 -12.844 -12.843 0.001

Mg 5.184e-004

Mg+2 4.977e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.512e-005 1.397e-005 -4.821 -4.855 -0.034

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 5.582e-007 5.589e-007 -6.253 -6.253 0.001

MgOH+ 9.716e-009 8.979e-009 -8.012 -8.047 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

NaCO3- 2.259e-010 2.087e-010 -9.646 -9.680 -0.034

NaOH 8.219e-013 8.230e-013 -12.085 -12.085 0.001

O(0) 3.801e-004

O2 1.901e-004 1.903e-004 -3.721 -3.721 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.770e-010 4.408e-010 -9.321 -9.356 -0.034

CaHSO4+ 5.424e-012 5.012e-012 -11.266 -11.300 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.48 -8.77 -8.29 CaCO3

Calcite -0.33 -8.77 -8.44 CaCO3

CO2(g) -1.83 -3.21 -1.37 CO2

Dolomite -1.04 -17.95 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.26 -25.38 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 45. 29/8/2012 22:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.770e-004 3.770e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551906e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0063 0.8077

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.770e-004

O2 1.885e-004 1.887e-004 -3.725 -3.724 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 46. 29/8/2012 23:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.776e-004 3.776e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99896

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.170e-003

Total CO2 (mol/kg) = 4.170e-003

Temperature (deg C) = 17.400

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551906e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0152 0.8080

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.891e-008 9.130e-008 -7.005 -7.040 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.170e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.050e-004 5.056e-004 -3.297 -3.296 0.001

CaHCO3+ 3.794e-005 3.513e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.056e-006 3.060e-006 -5.515 -5.514 0.001

CO3-2 2.983e-006 2.195e-006 -5.525 -5.659 -0.133

MgCO3 6.834e-007 6.843e-007 -6.165 -6.165 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.756e-010 2.547e-010 -9.560 -9.594 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.794e-005 3.513e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.056e-006 3.060e-006 -5.515 -5.514 0.001

CaOH+ 2.818e-009 2.604e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.400e-012 4.066e-012 -11.357 -11.391 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.549e-026

H2 2.774e-026 2.778e-026 -25.557 -25.556 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

MgCO3 6.834e-007 6.843e-007 -6.165 -6.165 0.001

MgOH+ 1.184e-008 1.094e-008 -7.927 -7.961 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.756e-010 2.547e-010 -9.560 -9.594 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.776e-004

O2 1.888e-004 1.891e-004 -3.724 -3.723 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

HSO4- 3.871e-010 3.577e-010 -9.412 -9.446 -0.034

CaHSO4+ 4.400e-012 4.066e-012 -11.357 -11.391 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.87 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 47. 29/8/2012 23:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.101e-004 4.101e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551909e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0155 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.101e-004

O2 2.051e-004 2.053e-004 -3.688 -3.688 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.69 -2.83 O2

Initial solution 48. 29/8/2012 23:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.245e-004 4.245e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99896

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.182e-003

Total CO2 (mol/kg) = 4.182e-003

Temperature (deg C) = 17.400

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551913e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0380 0.8093

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.666e-008 8.922e-008 -7.015 -7.050 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.182e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.168e-004 5.174e-004 -3.287 -3.286 0.001

CaHCO3+ 3.794e-005 3.514e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.987e-006 2.991e-006 -5.525 -5.524 0.001

CO3-2 2.916e-006 2.145e-006 -5.535 -5.669 -0.133

MgCO3 6.680e-007 6.688e-007 -6.175 -6.175 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.693e-010 2.489e-010 -9.570 -9.604 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.794e-005 3.514e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 2.987e-006 2.991e-006 -5.525 -5.524 0.001

CaOH+ 2.753e-009 2.545e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.503e-012 4.161e-012 -11.347 -11.381 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.810e-026

H2 2.905e-026 2.909e-026 -25.537 -25.536 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

MgCO3 6.680e-007 6.688e-007 -6.175 -6.175 0.001

MgOH+ 1.157e-008 1.069e-008 -7.937 -7.971 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.693e-010 2.489e-010 -9.570 -9.604 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 4.245e-004

O2 2.123e-004 2.125e-004 -3.673 -3.673 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

HSO4- 3.961e-010 3.660e-010 -9.402 -9.436 -0.034

CaHSO4+ 4.503e-012 4.161e-012 -11.347 -11.381 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.89 -17.80 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.67 -2.83 O2

Initial solution 49. 29/8/2012 23:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.026e-004 4.026e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551908e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0135 0.8081

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.026e-004

O2 2.013e-004 2.016e-004 -3.696 -3.696 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 50. 30/8/2012 00:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.408e-004 4.408e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99896

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.182e-003

Total CO2 (mol/kg) = 4.182e-003

Temperature (deg C) = 17.400

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551915e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0420 0.8095

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.666e-008 8.922e-008 -7.015 -7.050 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.182e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.168e-004 5.174e-004 -3.287 -3.286 0.001

CaHCO3+ 3.794e-005 3.514e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.987e-006 2.991e-006 -5.525 -5.524 0.001

CO3-2 2.916e-006 2.145e-006 -5.535 -5.669 -0.133

MgCO3 6.680e-007 6.688e-007 -6.175 -6.175 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.693e-010 2.489e-010 -9.570 -9.604 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.794e-005 3.514e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 2.987e-006 2.991e-006 -5.525 -5.524 0.001

CaOH+ 2.753e-009 2.545e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.503e-012 4.161e-012 -11.347 -11.381 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.810e-026

H2 2.905e-026 2.909e-026 -25.537 -25.536 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

MgCO3 6.680e-007 6.688e-007 -6.175 -6.175 0.001

MgOH+ 1.157e-008 1.069e-008 -7.937 -7.971 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.693e-010 2.489e-010 -9.570 -9.604 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 4.408e-004

O2 2.204e-004 2.207e-004 -3.657 -3.656 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

HSO4- 3.961e-010 3.660e-010 -9.402 -9.436 -0.034

CaHSO4+ 4.503e-012 4.161e-012 -11.347 -11.381 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.89 -17.80 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.82 -3.66 -2.83 O2

Initial solution 51. 30/8/2012 00:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.707e-004 3.707e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551908e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0145 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.159e-004 5.165e-004 -3.287 -3.287 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CO3-2 2.923e-006 2.150e-006 -5.534 -5.668 -0.133

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CaOH+ 2.753e-009 2.544e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 3.707e-004

O2 1.854e-004 1.856e-004 -3.732 -3.731 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.968e-010 3.667e-010 -9.401 -9.436 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.90 -3.73 -2.83 O2

Initial solution 52. 30/8/2012 00:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.714e-004 3.714e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551908e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0147 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.159e-004 5.165e-004 -3.287 -3.287 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CO3-2 2.923e-006 2.150e-006 -5.534 -5.668 -0.133

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CaOH+ 2.753e-009 2.544e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 3.714e-004

O2 1.857e-004 1.859e-004 -3.731 -3.731 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.968e-010 3.667e-010 -9.401 -9.436 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.90 -3.73 -2.83 O2

Initial solution 53. 30/8/2012 00:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.214e-004 4.214e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99896

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.182e-003

Total CO2 (mol/kg) = 4.182e-003

Temperature (deg C) = 17.400

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551913e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0372 0.8092

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.666e-008 8.922e-008 -7.015 -7.050 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.182e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.168e-004 5.174e-004 -3.287 -3.286 0.001

CaHCO3+ 3.794e-005 3.514e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.987e-006 2.991e-006 -5.525 -5.524 0.001

CO3-2 2.916e-006 2.145e-006 -5.535 -5.669 -0.133

MgCO3 6.680e-007 6.688e-007 -6.175 -6.175 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.693e-010 2.489e-010 -9.570 -9.604 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.794e-005 3.514e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 2.987e-006 2.991e-006 -5.525 -5.524 0.001

CaOH+ 2.753e-009 2.545e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.503e-012 4.161e-012 -11.347 -11.381 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.810e-026

H2 2.905e-026 2.909e-026 -25.537 -25.536 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

MgCO3 6.680e-007 6.688e-007 -6.175 -6.175 0.001

MgOH+ 1.157e-008 1.069e-008 -7.937 -7.971 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.693e-010 2.489e-010 -9.570 -9.604 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 4.214e-004

O2 2.107e-004 2.110e-004 -3.676 -3.676 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

HSO4- 3.961e-010 3.660e-010 -9.402 -9.436 -0.034

CaHSO4+ 4.503e-012 4.161e-012 -11.347 -11.381 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.89 -17.80 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.68 -2.83 O2

Initial solution 54. 30/8/2012 01:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.945e-004 3.945e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551908e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0113 0.8080

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.945e-004

O2 1.972e-004 1.975e-004 -3.705 -3.704 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.70 -2.83 O2

Initial solution 55. 30/8/2012 01:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.782e-004 3.782e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551908e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0167 0.8083

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.159e-004 5.165e-004 -3.287 -3.287 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CO3-2 2.923e-006 2.150e-006 -5.534 -5.668 -0.133

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CaOH+ 2.753e-009 2.544e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 3.782e-004

O2 1.891e-004 1.894e-004 -3.723 -3.723 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.968e-010 3.667e-010 -9.401 -9.436 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 56. 30/8/2012 01:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.139e-004 4.139e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551910e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0165 0.8083

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.139e-004

O2 2.069e-004 2.072e-004 -3.684 -3.684 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.68 -2.83 O2

Initial solution 57. 30/8/2012 01:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.857e-004 3.857e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551909e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0188 0.8084

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.159e-004 5.165e-004 -3.287 -3.287 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CO3-2 2.923e-006 2.150e-006 -5.534 -5.668 -0.133

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CaOH+ 2.753e-009 2.544e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 3.857e-004

O2 1.929e-004 1.931e-004 -3.715 -3.714 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.968e-010 3.667e-010 -9.401 -9.436 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 58. 30/8/2012 02:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.714e-004 3.714e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0047 0.8076

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.714e-004

O2 1.857e-004 1.859e-004 -3.731 -3.731 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.90 -3.73 -2.83 O2

Initial solution 59. 30/8/2012 02:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.220e-004 4.220e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99896

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.170e-003

Total CO2 (mol/kg) = 4.170e-003

Temperature (deg C) = 17.400

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0273 0.8086

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.891e-008 9.130e-008 -7.005 -7.040 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.170e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.050e-004 5.056e-004 -3.297 -3.296 0.001

CaHCO3+ 3.794e-005 3.513e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.056e-006 3.060e-006 -5.515 -5.514 0.001

CO3-2 2.983e-006 2.195e-006 -5.525 -5.659 -0.133

MgCO3 6.835e-007 6.843e-007 -6.165 -6.165 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.756e-010 2.547e-010 -9.560 -9.594 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.794e-005 3.513e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.056e-006 3.060e-006 -5.515 -5.514 0.001

CaOH+ 2.818e-009 2.604e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.400e-012 4.066e-012 -11.357 -11.391 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.549e-026

H2 2.774e-026 2.778e-026 -25.557 -25.556 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

MgCO3 6.835e-007 6.843e-007 -6.165 -6.165 0.001

MgOH+ 1.184e-008 1.094e-008 -7.927 -7.961 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.756e-010 2.547e-010 -9.560 -9.594 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.220e-004

O2 2.110e-004 2.113e-004 -3.676 -3.675 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

HSO4- 3.871e-010 3.577e-010 -9.412 -9.446 -0.034

CaHSO4+ 4.400e-012 4.066e-012 -11.357 -11.391 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.87 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.68 -2.83 O2

Initial solution 60. 30/8/2012 02:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.245e-004 4.245e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551913e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0292 0.8090

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.159e-004 5.165e-004 -3.287 -3.287 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CO3-2 2.923e-006 2.150e-006 -5.534 -5.668 -0.133

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CaOH+ 2.753e-009 2.544e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 4.245e-004

O2 2.123e-004 2.125e-004 -3.673 -3.673 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.968e-010 3.667e-010 -9.401 -9.436 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.67 -2.83 O2

Initial solution 61. 30/8/2012 02:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.820e-004 3.820e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99896

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.170e-003

Total CO2 (mol/kg) = 4.170e-003

Temperature (deg C) = 17.400

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551907e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0165 0.8080

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.891e-008 9.130e-008 -7.005 -7.040 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.170e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.050e-004 5.056e-004 -3.297 -3.296 0.001

CaHCO3+ 3.794e-005 3.513e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.056e-006 3.060e-006 -5.515 -5.514 0.001

CO3-2 2.983e-006 2.195e-006 -5.525 -5.659 -0.133

MgCO3 6.834e-007 6.843e-007 -6.165 -6.165 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.756e-010 2.547e-010 -9.560 -9.594 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.794e-005 3.513e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.056e-006 3.060e-006 -5.515 -5.514 0.001

CaOH+ 2.818e-009 2.604e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.400e-012 4.066e-012 -11.357 -11.391 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.549e-026

H2 2.774e-026 2.778e-026 -25.557 -25.556 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

MgCO3 6.834e-007 6.843e-007 -6.165 -6.165 0.001

MgOH+ 1.184e-008 1.094e-008 -7.927 -7.961 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.756e-010 2.547e-010 -9.560 -9.594 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.820e-004

O2 1.910e-004 1.912e-004 -3.719 -3.718 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

HSO4- 3.871e-010 3.577e-010 -9.412 -9.446 -0.034

CaHSO4+ 4.400e-012 4.066e-012 -11.357 -11.391 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.87 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 62. 30/8/2012 03:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.826e-004 3.826e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99896

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.170e-003

Total CO2 (mol/kg) = 4.170e-003

Temperature (deg C) = 17.400

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551907e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0167 0.8080

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.891e-008 9.130e-008 -7.005 -7.040 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.170e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.050e-004 5.056e-004 -3.297 -3.296 0.001

CaHCO3+ 3.794e-005 3.513e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.056e-006 3.060e-006 -5.515 -5.514 0.001

CO3-2 2.983e-006 2.195e-006 -5.525 -5.659 -0.133

MgCO3 6.834e-007 6.843e-007 -6.165 -6.165 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.756e-010 2.547e-010 -9.560 -9.594 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.794e-005 3.513e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.056e-006 3.060e-006 -5.515 -5.514 0.001

CaOH+ 2.818e-009 2.604e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.400e-012 4.066e-012 -11.357 -11.391 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.549e-026

H2 2.774e-026 2.778e-026 -25.557 -25.556 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

MgCO3 6.834e-007 6.843e-007 -6.165 -6.165 0.001

MgOH+ 1.184e-008 1.094e-008 -7.927 -7.961 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.756e-010 2.547e-010 -9.560 -9.594 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.826e-004

O2 1.913e-004 1.916e-004 -3.718 -3.718 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

HSO4- 3.871e-010 3.577e-010 -9.412 -9.446 -0.034

CaHSO4+ 4.400e-012 4.066e-012 -11.357 -11.391 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.87 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.72 -2.83 O2

Initial solution 63. 30/8/2012 03:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.089e-004 4.089e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551909e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0152 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.089e-004

O2 2.044e-004 2.047e-004 -3.689 -3.689 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.69 -2.83 O2

Initial solution 64. 30/8/2012 03:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.814e-004 3.814e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.140

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.634e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.273e-003

Total CO2 (mol/kg) = 4.273e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551927e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0876 0.8124

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.295e-008 7.656e-008 -7.081 -7.116 -0.035

H+ 7.779e-008 7.244e-008 -7.109 -7.140 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.273e-003

HCO3- 3.608e-003 3.341e-003 -2.443 -2.476 -0.033

CO2 6.064e-004 6.072e-004 -3.217 -3.217 0.001

CaHCO3+ 3.805e-005 3.524e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.512e-005 1.397e-005 -4.821 -4.855 -0.034

CaCO3 2.554e-006 2.557e-006 -5.593 -5.592 0.001

CO3-2 2.489e-006 1.831e-006 -5.604 -5.737 -0.133

MgCO3 5.711e-007 5.719e-007 -6.243 -6.243 0.001

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaCO3- 2.311e-010 2.136e-010 -9.636 -9.670 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.457e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.805e-005 3.524e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

CaCO3 2.554e-006 2.557e-006 -5.593 -5.592 0.001

CaOH+ 2.344e-009 2.166e-009 -8.630 -8.664 -0.034

CaHSO4+ 5.300e-012 4.898e-012 -11.276 -11.310 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 8.012e-026

H2 4.006e-026 4.011e-026 -25.397 -25.397 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.467e-013 1.469e-013 -12.834 -12.833 0.001

Mg 5.184e-004

Mg+2 4.977e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.512e-005 1.397e-005 -4.821 -4.855 -0.034

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 5.711e-007 5.719e-007 -6.243 -6.243 0.001

MgOH+ 9.943e-009 9.188e-009 -8.003 -8.037 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

NaCO3- 2.311e-010 2.136e-010 -9.636 -9.670 -0.034

NaOH 8.411e-013 8.422e-013 -12.075 -12.075 0.001

O(0) 3.814e-004

O2 1.907e-004 1.909e-004 -3.720 -3.719 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.662e-010 4.308e-010 -9.331 -9.366 -0.034

CaHSO4+ 5.300e-012 4.898e-012 -11.276 -11.310 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.47 -8.76 -8.29 CaCO3

Calcite -0.32 -8.76 -8.44 CaCO3

CO2(g) -1.84 -3.22 -1.37 CO2

Dolomite -1.02 -17.93 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.28 -25.40 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 65. 30/8/2012 03:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.045e-004 4.045e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.158e-003

Total CO2 (mol/kg) = 4.158e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0140 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.158e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.027e-004 5.034e-004 -3.299 -3.298 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.051e-006 3.055e-006 -5.516 -5.515 0.001

CO3-2 2.982e-006 2.194e-006 -5.526 -5.659 -0.133

MgCO3 6.845e-007 6.854e-007 -6.165 -6.164 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.770e-010 2.560e-010 -9.558 -9.592 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.051e-006 3.055e-006 -5.516 -5.515 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.399e-012 4.065e-012 -11.357 -11.391 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 6.845e-007 6.854e-007 -6.165 -6.164 0.001

MgOH+ 1.195e-008 1.105e-008 -7.922 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.770e-010 2.560e-010 -9.558 -9.592 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.045e-004

O2 2.023e-004 2.025e-004 -3.694 -3.694 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.879e-010 3.585e-010 -9.411 -9.445 -0.034

CaHSO4+ 4.399e-012 4.065e-012 -11.357 -11.391 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.87 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.69 -2.83 O2

Initial solution 66. 30/8/2012 04:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.064e-004 4.064e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551909e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0145 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.064e-004

O2 2.032e-004 2.035e-004 -3.692 -3.692 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.69 -2.83 O2

Initial solution 67. 30/8/2012 04:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.270e-004 4.270e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0199 0.8085

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.270e-004

O2 2.135e-004 2.138e-004 -3.671 -3.670 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.67 -2.83 O2

Initial solution 68. 30/8/2012 04:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.314e-004 4.314e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0210 0.8086

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.314e-004

O2 2.157e-004 2.160e-004 -3.666 -3.666 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.83 -3.67 -2.83 O2

Initial solution 69. 30/8/2012 04:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.007e-004 4.007e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.158e-003

Total CO2 (mol/kg) = 4.158e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551906e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0030 0.8075

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.158e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 4.926e-004 4.932e-004 -3.308 -3.307 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.138e-006 3.142e-006 -5.503 -5.503 0.001

CO3-2 3.060e-006 2.251e-006 -5.514 -5.648 -0.133

MgCO3 7.020e-007 7.029e-007 -6.154 -6.153 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.842e-010 2.626e-010 -9.546 -9.581 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.453e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.138e-006 3.142e-006 -5.503 -5.503 0.001

CaOH+ 2.883e-009 2.664e-009 -8.540 -8.574 -0.034

CaHSO4+ 4.307e-012 3.980e-012 -11.366 -11.400 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 7.020e-007 7.029e-007 -6.154 -6.153 0.001

MgOH+ 1.223e-008 1.130e-008 -7.913 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.842e-010 2.626e-010 -9.546 -9.581 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.007e-004

O2 2.004e-004 2.006e-004 -3.698 -3.698 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.790e-010 3.502e-010 -9.421 -9.456 -0.034

CaHSO4+ 4.307e-012 3.980e-012 -11.366 -11.400 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.84 -17.75 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 70. 30/8/2012 05:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.870e-004 3.870e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.170

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.622e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.220e-003

Total CO2 (mol/kg) = 4.220e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551916e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0592 0.8108

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.887e-008 8.204e-008 -7.051 -7.086 -0.035

H+ 7.259e-008 6.761e-008 -7.139 -7.170 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.220e-003

HCO3- 3.597e-003 3.331e-003 -2.444 -2.477 -0.033

CO2 5.643e-004 5.650e-004 -3.248 -3.248 0.001

CaHCO3+ 3.784e-005 3.504e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.508e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 2.721e-006 2.725e-006 -5.565 -5.565 0.001

CO3-2 2.658e-006 1.956e-006 -5.575 -5.709 -0.133

MgCO3 6.103e-007 6.111e-007 -6.214 -6.214 0.001

NaHCO3 1.728e-008 1.730e-008 -7.762 -7.762 0.001

NaCO3- 2.469e-010 2.282e-010 -9.607 -9.642 -0.034

Ca 1.336e-003

Ca+2 1.283e-003 9.433e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.784e-005 3.504e-005 -4.422 -4.455 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 2.721e-006 2.725e-006 -5.565 -5.565 0.001

CaOH+ 2.505e-009 2.315e-009 -8.601 -8.635 -0.034

CaHSO4+ 4.936e-012 4.562e-012 -11.307 -11.341 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.978e-026

H2 3.489e-026 3.494e-026 -25.457 -25.457 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.572e-013 1.574e-013 -12.804 -12.803 0.001

Mg 5.184e-004

Mg+2 4.977e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.508e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 6.103e-007 6.111e-007 -6.214 -6.214 0.001

MgOH+ 1.066e-008 9.848e-009 -7.972 -8.007 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.728e-008 1.730e-008 -7.762 -7.762 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.469e-010 2.282e-010 -9.607 -9.642 -0.034

NaOH 9.013e-013 9.025e-013 -12.045 -12.045 0.001

O(0) 3.870e-004

O2 1.935e-004 1.937e-004 -3.713 -3.713 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 4.353e-010 4.023e-010 -9.361 -9.395 -0.034

CaHSO4+ 4.936e-012 4.562e-012 -11.307 -11.341 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.44 -8.73 -8.29 CaCO3

Calcite -0.29 -8.73 -8.44 CaCO3

CO2(g) -1.87 -3.25 -1.37 CO2

Dolomite -0.97 -17.88 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.34 -25.46 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 71. 30/8/2012 05:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.020e-004 4.020e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.182e-003

Total CO2 (mol/kg) = 4.182e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551910e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0333 0.8093

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.523e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.182e-003

HCO3- 3.596e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.265e-004 5.272e-004 -3.279 -3.278 0.001

CaHCO3+ 3.782e-005 3.503e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 2.915e-006 2.919e-006 -5.535 -5.535 0.001

CO3-2 2.848e-006 2.096e-006 -5.545 -5.679 -0.133

MgCO3 6.538e-007 6.546e-007 -6.185 -6.184 0.001

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaCO3- 2.645e-010 2.445e-010 -9.578 -9.612 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.431e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.782e-005 3.503e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 2.915e-006 2.919e-006 -5.535 -5.535 0.001

CaOH+ 2.684e-009 2.480e-009 -8.571 -8.605 -0.034

CaHSO4+ 4.606e-012 4.257e-012 -11.337 -11.371 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.687e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 6.538e-007 6.546e-007 -6.185 -6.184 0.001

MgOH+ 1.142e-008 1.055e-008 -7.942 -7.977 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.645e-010 2.445e-010 -9.578 -9.612 -0.034

NaOH 9.658e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 4.020e-004

O2 2.010e-004 2.013e-004 -3.697 -3.696 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 4.062e-010 3.754e-010 -9.391 -9.425 -0.034

CaHSO4+ 4.606e-012 4.257e-012 -11.337 -11.371 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.91 -17.82 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 72. 30/8/2012 05:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.007e-004 4.007e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.160

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.622e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.233e-003

Total CO2 (mol/kg) = 4.233e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551920e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0730 0.8116

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.685e-008 8.017e-008 -7.061 -7.096 -0.035

H+ 7.428e-008 6.918e-008 -7.129 -7.160 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.233e-003

HCO3- 3.597e-003 3.331e-003 -2.444 -2.477 -0.033

CO2 5.775e-004 5.782e-004 -3.238 -3.238 0.001

CaHCO3+ 3.784e-005 3.505e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.508e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 2.660e-006 2.663e-006 -5.575 -5.575 0.001

CO3-2 2.598e-006 1.912e-006 -5.585 -5.719 -0.133

MgCO3 5.965e-007 5.973e-007 -6.224 -6.224 0.001

NaHCO3 1.728e-008 1.730e-008 -7.762 -7.762 0.001

NaCO3- 2.413e-010 2.230e-010 -9.617 -9.652 -0.034

Ca 1.336e-003

Ca+2 1.283e-003 9.433e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.784e-005 3.505e-005 -4.422 -4.455 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 2.660e-006 2.663e-006 -5.575 -5.575 0.001

CaOH+ 2.448e-009 2.263e-009 -8.611 -8.645 -0.034

CaHSO4+ 5.051e-012 4.668e-012 -11.297 -11.331 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 7.307e-026

H2 3.653e-026 3.658e-026 -25.437 -25.437 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.536e-013 1.538e-013 -12.814 -12.813 0.001

Mg 5.184e-004

Mg+2 4.977e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.508e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.059e-006 5.066e-006 -5.296 -5.295 0.001

MgCO3 5.965e-007 5.973e-007 -6.224 -6.224 0.001

MgOH+ 1.041e-008 9.624e-009 -7.982 -8.017 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.728e-008 1.730e-008 -7.762 -7.762 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.413e-010 2.230e-010 -9.617 -9.652 -0.034

NaOH 8.808e-013 8.819e-013 -12.055 -12.055 0.001

O(0) 4.007e-004

O2 2.004e-004 2.006e-004 -3.698 -3.698 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.059e-006 5.066e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 4.454e-010 4.116e-010 -9.351 -9.385 -0.034

CaHSO4+ 5.051e-012 4.668e-012 -11.297 -11.331 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.45 -8.74 -8.29 CaCO3

Calcite -0.30 -8.74 -8.44 CaCO3

CO2(g) -1.86 -3.24 -1.37 CO2

Dolomite -0.99 -17.90 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.32 -25.44 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 73. 30/8/2012 05:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.020e-004 4.020e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.250

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.123e-003

Total CO2 (mol/kg) = 4.123e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551898e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9833 0.8064

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.068e-007 9.863e-008 -6.971 -7.006 -0.035

H+ 6.038e-008 5.623e-008 -7.219 -7.250 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.123e-003

HCO3- 3.594e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.690e-004 4.697e-004 -3.329 -3.328 0.001

CaHCO3+ 3.780e-005 3.501e-005 -4.423 -4.456 -0.033

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.268e-006 3.273e-006 -5.486 -5.485 0.001

CO3-2 3.194e-006 2.350e-006 -5.496 -5.629 -0.133

MgCO3 7.332e-007 7.341e-007 -6.135 -6.134 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.967e-010 2.742e-010 -9.528 -9.562 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.780e-005 3.501e-005 -4.423 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.268e-006 3.273e-006 -5.486 -5.485 0.001

CaOH+ 3.011e-009 2.782e-009 -8.521 -8.556 -0.034

CaHSO4+ 4.104e-012 3.793e-012 -11.387 -11.421 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 4.828e-026

H2 2.414e-026 2.417e-026 -25.617 -25.617 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.890e-013 1.892e-013 -12.724 -12.723 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.332e-007 7.341e-007 -6.135 -6.134 0.001

MgOH+ 1.281e-008 1.184e-008 -7.892 -7.927 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.967e-010 2.742e-010 -9.528 -9.562 -0.034

NaOH 1.084e-012 1.085e-012 -11.965 -11.965 0.001

O(0) 4.020e-004

O2 2.010e-004 2.013e-004 -3.697 -3.696 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.621e-010 3.346e-010 -9.441 -9.475 -0.034

CaHSO4+ 4.104e-012 3.793e-012 -11.387 -11.421 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.36 -8.65 -8.29 CaCO3

Calcite -0.21 -8.65 -8.44 CaCO3

CO2(g) -1.95 -3.33 -1.37 CO2

Dolomite -0.81 -17.72 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.50 -25.62 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 74. 30/8/2012 06:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.189e-004 4.189e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9978 0.8072

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.044e-007 9.639e-008 -6.981 -7.016 -0.035

H+ 6.179e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.605e-003 3.338e-003 -2.443 -2.476 -0.033

CO2 4.813e-004 4.819e-004 -3.318 -3.317 0.001

CaHCO3+ 3.800e-005 3.519e-005 -4.420 -4.454 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.211e-006 3.215e-006 -5.493 -5.493 0.001

CO3-2 3.131e-006 2.303e-006 -5.504 -5.638 -0.133

MgCO3 7.183e-007 7.192e-007 -6.144 -6.143 0.001

NaHCO3 1.731e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.908e-010 2.687e-010 -9.536 -9.571 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.453e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.800e-005 3.519e-005 -4.420 -4.454 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.211e-006 3.215e-006 -5.493 -5.493 0.001

CaOH+ 2.950e-009 2.726e-009 -8.530 -8.564 -0.034

CaHSO4+ 4.209e-012 3.889e-012 -11.376 -11.410 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.055e-026

H2 2.528e-026 2.531e-026 -25.597 -25.597 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 7.183e-007 7.192e-007 -6.144 -6.143 0.001

MgOH+ 1.251e-008 1.156e-008 -7.903 -7.937 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.731e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.908e-010 2.687e-010 -9.536 -9.571 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 4.189e-004

O2 2.094e-004 2.097e-004 -3.679 -3.678 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.703e-010 3.422e-010 -9.431 -9.466 -0.034

CaHSO4+ 4.209e-012 3.889e-012 -11.376 -11.410 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.37 CO2

Dolomite -0.82 -17.73 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.68 -2.83 O2

Initial solution 75. 30/8/2012 06:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.957e-004 3.957e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.158e-003

Total CO2 (mol/kg) = 4.158e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0116 0.8080

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.158e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.027e-004 5.034e-004 -3.299 -3.298 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.051e-006 3.055e-006 -5.516 -5.515 0.001

CO3-2 2.982e-006 2.194e-006 -5.526 -5.659 -0.133

MgCO3 6.845e-007 6.854e-007 -6.165 -6.164 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.770e-010 2.560e-010 -9.558 -9.592 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.051e-006 3.055e-006 -5.516 -5.515 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.399e-012 4.065e-012 -11.357 -11.391 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 6.845e-007 6.854e-007 -6.165 -6.164 0.001

MgOH+ 1.195e-008 1.105e-008 -7.922 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.770e-010 2.560e-010 -9.558 -9.592 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.957e-004

O2 1.979e-004 1.981e-004 -3.704 -3.703 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.879e-010 3.585e-010 -9.411 -9.445 -0.034

CaHSO4+ 4.399e-012 4.065e-012 -11.357 -11.391 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.87 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.70 -2.83 O2

Initial solution 76. 30/8/2012 06:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.151e-004 4.151e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.135e-003

Total CO2 (mol/kg) = 4.135e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551902e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9968 0.8072

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.044e-007 9.639e-008 -6.981 -7.016 -0.035

H+ 6.179e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.135e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.800e-004 4.806e-004 -3.319 -3.318 0.001

CaHCO3+ 3.780e-005 3.501e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.194e-006 3.198e-006 -5.496 -5.495 0.001

CO3-2 3.122e-006 2.297e-006 -5.506 -5.639 -0.133

MgCO3 7.166e-007 7.175e-007 -6.145 -6.144 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.780e-005 3.501e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.194e-006 3.198e-006 -5.496 -5.495 0.001

CaOH+ 2.942e-009 2.719e-009 -8.531 -8.566 -0.034

CaHSO4+ 4.200e-012 3.882e-012 -11.377 -11.411 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.055e-026

H2 2.528e-026 2.531e-026 -25.597 -25.597 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.166e-007 7.175e-007 -6.145 -6.144 0.001

MgOH+ 1.252e-008 1.157e-008 -7.902 -7.937 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 4.151e-004

O2 2.076e-004 2.078e-004 -3.683 -3.682 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.705e-010 3.424e-010 -9.431 -9.465 -0.034

CaHSO4+ 4.200e-012 3.882e-012 -11.377 -11.411 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.37 CO2

Dolomite -0.83 -17.74 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.68 -2.83 O2

Initial solution 77. 30/8/2012 06:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.695e-004 3.695e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.182e-003

Total CO2 (mol/kg) = 4.182e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551907e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0242 0.8087

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.523e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.182e-003

HCO3- 3.596e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.265e-004 5.272e-004 -3.279 -3.278 0.001

CaHCO3+ 3.782e-005 3.503e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 2.915e-006 2.919e-006 -5.535 -5.535 0.001

CO3-2 2.848e-006 2.096e-006 -5.545 -5.679 -0.133

MgCO3 6.538e-007 6.546e-007 -6.185 -6.184 0.001

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaCO3- 2.645e-010 2.445e-010 -9.578 -9.612 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.431e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.782e-005 3.503e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 2.915e-006 2.919e-006 -5.535 -5.535 0.001

CaOH+ 2.684e-009 2.480e-009 -8.571 -8.605 -0.034

CaHSO4+ 4.606e-012 4.257e-012 -11.337 -11.371 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.687e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 6.538e-007 6.546e-007 -6.185 -6.184 0.001

MgOH+ 1.142e-008 1.055e-008 -7.942 -7.977 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.645e-010 2.445e-010 -9.578 -9.612 -0.034

NaOH 9.658e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 3.695e-004

O2 1.847e-004 1.850e-004 -3.733 -3.733 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 4.062e-010 3.754e-010 -9.391 -9.425 -0.034

CaHSO4+ 4.606e-012 4.257e-012 -11.337 -11.371 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.91 -17.82 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.90 -3.73 -2.83 O2

Initial solution 78. 30/8/2012 07:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.832e-004 3.832e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551906e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0181 0.8084

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.596e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.145e-004 5.151e-004 -3.289 -3.288 0.001

CaHCO3+ 3.782e-005 3.503e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 2.982e-006 2.986e-006 -5.525 -5.525 0.001

CO3-2 2.914e-006 2.144e-006 -5.536 -5.669 -0.133

MgCO3 6.690e-007 6.698e-007 -6.175 -6.174 0.001

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaCO3- 2.707e-010 2.502e-010 -9.568 -9.602 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.431e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.782e-005 3.503e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 2.982e-006 2.986e-006 -5.525 -5.525 0.001

CaOH+ 2.746e-009 2.538e-009 -8.561 -8.595 -0.034

CaHSO4+ 4.501e-012 4.160e-012 -11.347 -11.381 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.724e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 6.690e-007 6.698e-007 -6.175 -6.174 0.001

MgOH+ 1.168e-008 1.080e-008 -7.932 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.707e-010 2.502e-010 -9.568 -9.602 -0.034

NaOH 9.883e-013 9.896e-013 -12.005 -12.005 0.001

O(0) 3.832e-004

O2 1.916e-004 1.919e-004 -3.718 -3.717 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.970e-010 3.669e-010 -9.401 -9.435 -0.034

CaHSO4+ 4.501e-012 4.160e-012 -11.347 -11.381 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.89 -17.80 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.72 -2.83 O2

Initial solution 79. 30/8/2012 07:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.982e-004 3.982e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.158e-003

Total CO2 (mol/kg) = 4.158e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0123 0.8081

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.158e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.027e-004 5.034e-004 -3.299 -3.298 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.051e-006 3.055e-006 -5.516 -5.515 0.001

CO3-2 2.982e-006 2.194e-006 -5.526 -5.659 -0.133

MgCO3 6.845e-007 6.854e-007 -6.165 -6.164 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.770e-010 2.560e-010 -9.558 -9.592 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.051e-006 3.055e-006 -5.516 -5.515 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.399e-012 4.065e-012 -11.357 -11.391 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 6.845e-007 6.854e-007 -6.165 -6.164 0.001

MgOH+ 1.195e-008 1.105e-008 -7.922 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.770e-010 2.560e-010 -9.558 -9.592 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.982e-004

O2 1.991e-004 1.994e-004 -3.701 -3.700 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.879e-010 3.585e-010 -9.411 -9.445 -0.034

CaHSO4+ 4.399e-012 4.065e-012 -11.357 -11.391 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.87 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.70 -2.83 O2

Initial solution 80. 30/8/2012 07:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.882e-004 3.882e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551901e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9995 0.8073

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.882e-004

O2 1.941e-004 1.944e-004 -3.712 -3.711 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 81. 30/8/2012 07:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.651e-004 3.651e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.135e-003

Total CO2 (mol/kg) = 4.135e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551897e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9829 0.8064

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.044e-007 9.639e-008 -6.981 -7.016 -0.035

H+ 6.179e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.135e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.800e-004 4.806e-004 -3.319 -3.318 0.001

CaHCO3+ 3.780e-005 3.501e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.194e-006 3.198e-006 -5.496 -5.495 0.001

CO3-2 3.122e-006 2.297e-006 -5.506 -5.639 -0.133

MgCO3 7.166e-007 7.175e-007 -6.145 -6.144 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.780e-005 3.501e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.194e-006 3.198e-006 -5.496 -5.495 0.001

CaOH+ 2.942e-009 2.719e-009 -8.531 -8.566 -0.034

CaHSO4+ 4.200e-012 3.882e-012 -11.377 -11.411 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.055e-026

H2 2.528e-026 2.531e-026 -25.597 -25.597 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.166e-007 7.175e-007 -6.145 -6.144 0.001

MgOH+ 1.252e-008 1.157e-008 -7.902 -7.937 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 3.651e-004

O2 1.826e-004 1.828e-004 -3.739 -3.738 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.705e-010 3.424e-010 -9.431 -9.465 -0.034

CaHSO4+ 4.200e-012 3.882e-012 -11.377 -11.411 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.37 CO2

Dolomite -0.83 -17.74 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.90 -3.74 -2.83 O2

Initial solution 82. 30/8/2012 08:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.939e-004 3.939e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551902e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0011 0.8074

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.939e-004

O2 1.969e-004 1.972e-004 -3.706 -3.705 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.71 -2.83 O2

Initial solution 83. 30/8/2012 08:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.864e-004 3.864e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.135e-003

Total CO2 (mol/kg) = 4.135e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551899e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9890 0.8067

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.044e-007 9.639e-008 -6.981 -7.016 -0.035

H+ 6.179e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.135e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.800e-004 4.806e-004 -3.319 -3.318 0.001

CaHCO3+ 3.780e-005 3.501e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.194e-006 3.198e-006 -5.496 -5.495 0.001

CO3-2 3.122e-006 2.297e-006 -5.506 -5.639 -0.133

MgCO3 7.166e-007 7.175e-007 -6.145 -6.144 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.780e-005 3.501e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.194e-006 3.198e-006 -5.496 -5.495 0.001

CaOH+ 2.942e-009 2.719e-009 -8.531 -8.566 -0.034

CaHSO4+ 4.200e-012 3.882e-012 -11.377 -11.411 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.055e-026

H2 2.528e-026 2.531e-026 -25.597 -25.597 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.166e-007 7.175e-007 -6.145 -6.144 0.001

MgOH+ 1.252e-008 1.157e-008 -7.902 -7.937 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 3.864e-004

O2 1.932e-004 1.934e-004 -3.714 -3.713 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.705e-010 3.424e-010 -9.431 -9.465 -0.034

CaHSO4+ 4.200e-012 3.882e-012 -11.377 -11.411 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.37 CO2

Dolomite -0.83 -17.74 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 84. 30/8/2012 08:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.726e-004 3.726e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.135e-003

Total CO2 (mol/kg) = 4.135e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551897e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9851 0.8065

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.044e-007 9.639e-008 -6.981 -7.016 -0.035

H+ 6.179e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.135e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.800e-004 4.806e-004 -3.319 -3.318 0.001

CaHCO3+ 3.780e-005 3.501e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.194e-006 3.198e-006 -5.496 -5.495 0.001

CO3-2 3.122e-006 2.297e-006 -5.506 -5.639 -0.133

MgCO3 7.166e-007 7.175e-007 -6.145 -6.144 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.780e-005 3.501e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.194e-006 3.198e-006 -5.496 -5.495 0.001

CaOH+ 2.942e-009 2.719e-009 -8.531 -8.566 -0.034

CaHSO4+ 4.200e-012 3.882e-012 -11.377 -11.411 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.055e-026

H2 2.528e-026 2.531e-026 -25.597 -25.597 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.166e-007 7.175e-007 -6.145 -6.144 0.001

MgOH+ 1.252e-008 1.157e-008 -7.902 -7.937 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 3.726e-004

O2 1.863e-004 1.865e-004 -3.730 -3.729 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.705e-010 3.424e-010 -9.431 -9.465 -0.034

CaHSO4+ 4.200e-012 3.882e-012 -11.377 -11.411 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.37 CO2

Dolomite -0.83 -17.74 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.90 -3.73 -2.83 O2

Initial solution 85. 30/8/2012 08:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.714e-004 3.714e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551900e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9947 0.8070

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.714e-004

O2 1.857e-004 1.859e-004 -3.731 -3.731 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.90 -3.73 -2.83 O2

Initial solution 86. 30/8/2012 09:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.145e-004 4.145e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0066 0.8077

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.145e-004

O2 2.073e-004 2.075e-004 -3.684 -3.683 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.68 -2.83 O2

Initial solution 87. 30/8/2012 09:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.151e-004 4.151e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0068 0.8077

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.151e-004

O2 2.076e-004 2.078e-004 -3.683 -3.682 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.68 -2.83 O2

Initial solution 88. 30/8/2012 09:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.026e-004 4.026e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551903e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0035 0.8076

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.026e-004

O2 2.013e-004 2.016e-004 -3.696 -3.696 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 89. 30/8/2012 09:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.832e-004 3.832e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551901e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9981 0.8072

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.832e-004

O2 1.916e-004 1.919e-004 -3.718 -3.717 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.72 -2.83 O2

Initial solution 90. 30/8/2012 10:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.620e-004 3.620e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551899e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9919 0.8069

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.620e-004

O2 1.810e-004 1.812e-004 -3.742 -3.742 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.91 -3.74 -2.83 O2

Initial solution 91. 30/8/2012 10:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.001e-004 4.001e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551903e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0028 0.8075

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.001e-004

O2 2.001e-004 2.003e-004 -3.699 -3.698 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 92. 30/8/2012 10:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.776e-004 3.776e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551900e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9965 0.8072

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.776e-004

O2 1.888e-004 1.891e-004 -3.724 -3.723 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 93. 30/8/2012 10:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.782e-004 3.782e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.145e-003

Total CO2 (mol/kg) = 4.145e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551900e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9880 0.8069

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.029e-007 9.497e-008 -6.988 -7.022 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.145e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.904e-004 4.910e-004 -3.309 -3.309 0.001

CaHCO3+ 3.788e-005 3.508e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.134e-006 3.138e-006 -5.504 -5.503 0.001

CO3-2 3.058e-006 2.250e-006 -5.515 -5.648 -0.133

MgCO3 7.030e-007 7.039e-007 -6.153 -6.152 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.856e-010 2.639e-010 -9.544 -9.579 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.788e-005 3.508e-005 -4.422 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.134e-006 3.138e-006 -5.504 -5.503 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.306e-012 3.979e-012 -11.366 -11.400 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.288e-026

H2 2.644e-026 2.647e-026 -25.578 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 7.030e-007 7.039e-007 -6.153 -6.152 0.001

MgOH+ 1.235e-008 1.141e-008 -7.908 -7.943 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.856e-010 2.639e-010 -9.544 -9.579 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.782e-004

O2 1.891e-004 1.894e-004 -3.723 -3.723 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.798e-010 3.510e-010 -9.420 -9.455 -0.034

CaHSO4+ 4.306e-012 3.979e-012 -11.366 -11.400 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 94. 30/8/2012 11:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.895e-004 3.895e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.157e-003

Total CO2 (mol/kg) = 4.157e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0012 0.8077

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.005e-007 9.281e-008 -6.998 -7.032 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.157e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.019e-004 5.025e-004 -3.299 -3.299 0.001

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CO3-2 2.989e-006 2.199e-006 -5.524 -5.658 -0.133

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.537e-026

H2 2.769e-026 2.772e-026 -25.558 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

MgOH+ 1.207e-008 1.115e-008 -7.918 -7.953 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.895e-004

O2 1.947e-004 1.950e-004 -3.711 -3.710 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.886e-010 3.592e-010 -9.410 -9.445 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 95. 30/8/2012 11:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.901e-004 3.901e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.156e-003

Total CO2 (mol/kg) = 4.156e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551903e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9926 0.8075

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.014e-007 9.357e-008 -6.994 -7.029 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.156e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.010e-004 5.016e-004 -3.300 -3.300 0.001

CaHCO3+ 3.796e-005 3.516e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.074e-006 3.078e-006 -5.512 -5.512 0.001

CO3-2 2.996e-006 2.204e-006 -5.523 -5.657 -0.133

MgCO3 6.898e-007 6.906e-007 -6.161 -6.161 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.813e-010 2.599e-010 -9.551 -9.585 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.796e-005 3.516e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.074e-006 3.078e-006 -5.512 -5.512 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.413e-012 4.079e-012 -11.355 -11.389 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.531e-026

H2 2.766e-026 2.769e-026 -25.558 -25.558 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 6.898e-007 6.906e-007 -6.161 -6.161 0.001

MgOH+ 1.218e-008 1.126e-008 -7.914 -7.949 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.466 -8.500 -0.034

NaCO3- 2.813e-010 2.599e-010 -9.551 -9.585 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.901e-004

O2 1.951e-004 1.953e-004 -3.710 -3.709 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.466 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.894e-010 3.598e-010 -9.410 -9.444 -0.034

CaHSO4+ 4.413e-012 4.079e-012 -11.355 -11.389 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.77 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.87 -3.71 -2.84 O2

Initial solution 96. 30/8/2012 11:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.032e-004 4.032e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.157e-003

Total CO2 (mol/kg) = 4.157e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0049 0.8079

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.005e-007 9.281e-008 -6.998 -7.032 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.157e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.019e-004 5.025e-004 -3.299 -3.299 0.001

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CO3-2 2.989e-006 2.199e-006 -5.524 -5.658 -0.133

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.537e-026

H2 2.769e-026 2.772e-026 -25.558 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

MgOH+ 1.207e-008 1.115e-008 -7.918 -7.953 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.032e-004

O2 2.016e-004 2.019e-004 -3.695 -3.695 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.886e-010 3.592e-010 -9.410 -9.445 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.69 -2.83 O2

Initial solution 97. 30/8/2012 11:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.976e-004 3.976e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.156e-003

Total CO2 (mol/kg) = 4.156e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9947 0.8076

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.014e-007 9.357e-008 -6.994 -7.029 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.156e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.010e-004 5.016e-004 -3.300 -3.300 0.001

CaHCO3+ 3.796e-005 3.516e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.074e-006 3.078e-006 -5.512 -5.512 0.001

CO3-2 2.996e-006 2.204e-006 -5.523 -5.657 -0.133

MgCO3 6.898e-007 6.906e-007 -6.161 -6.161 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.813e-010 2.599e-010 -9.551 -9.585 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.796e-005 3.516e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.074e-006 3.078e-006 -5.512 -5.512 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.413e-012 4.079e-012 -11.355 -11.389 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.531e-026

H2 2.766e-026 2.769e-026 -25.558 -25.558 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 6.898e-007 6.906e-007 -6.161 -6.161 0.001

MgOH+ 1.218e-008 1.126e-008 -7.914 -7.949 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.466 -8.500 -0.034

NaCO3- 2.813e-010 2.599e-010 -9.551 -9.585 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.976e-004

O2 1.988e-004 1.991e-004 -3.702 -3.701 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.466 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.894e-010 3.598e-010 -9.410 -9.444 -0.034

CaHSO4+ 4.413e-012 4.079e-012 -11.355 -11.389 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.77 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.87 -3.70 -2.84 O2

Initial solution 98. 30/8/2012 12:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.820e-004 3.820e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.156e-003

Total CO2 (mol/kg) = 4.156e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551903e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9904 0.8074

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.014e-007 9.357e-008 -6.994 -7.029 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.156e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.010e-004 5.016e-004 -3.300 -3.300 0.001

CaHCO3+ 3.796e-005 3.516e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.074e-006 3.078e-006 -5.512 -5.512 0.001

CO3-2 2.996e-006 2.204e-006 -5.523 -5.657 -0.133

MgCO3 6.898e-007 6.906e-007 -6.161 -6.161 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.813e-010 2.599e-010 -9.551 -9.585 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.796e-005 3.516e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.074e-006 3.078e-006 -5.512 -5.512 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.413e-012 4.079e-012 -11.355 -11.389 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.531e-026

H2 2.766e-026 2.769e-026 -25.558 -25.558 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 6.898e-007 6.906e-007 -6.161 -6.161 0.001

MgOH+ 1.218e-008 1.126e-008 -7.914 -7.949 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.466 -8.500 -0.034

NaCO3- 2.813e-010 2.599e-010 -9.551 -9.585 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.820e-004

O2 1.910e-004 1.912e-004 -3.719 -3.718 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.466 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.894e-010 3.598e-010 -9.410 -9.444 -0.034

CaHSO4+ 4.413e-012 4.079e-012 -11.355 -11.389 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.77 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.88 -3.72 -2.84 O2

Initial solution 99. 30/8/2012 12:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.058e-004 4.058e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.156e-003

Total CO2 (mol/kg) = 4.156e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9969 0.8077

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.014e-007 9.357e-008 -6.994 -7.029 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.156e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.010e-004 5.016e-004 -3.300 -3.300 0.001

CaHCO3+ 3.796e-005 3.516e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.074e-006 3.078e-006 -5.512 -5.512 0.001

CO3-2 2.996e-006 2.204e-006 -5.523 -5.657 -0.133

MgCO3 6.898e-007 6.906e-007 -6.161 -6.161 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.813e-010 2.599e-010 -9.551 -9.585 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.796e-005 3.516e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.074e-006 3.078e-006 -5.512 -5.512 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.413e-012 4.079e-012 -11.355 -11.389 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.531e-026

H2 2.766e-026 2.769e-026 -25.558 -25.558 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 6.898e-007 6.906e-007 -6.161 -6.161 0.001

MgOH+ 1.218e-008 1.126e-008 -7.914 -7.949 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.466 -8.500 -0.034

NaCO3- 2.813e-010 2.599e-010 -9.551 -9.585 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.058e-004

O2 2.029e-004 2.031e-004 -3.693 -3.692 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.466 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.894e-010 3.598e-010 -9.410 -9.444 -0.034

CaHSO4+ 4.413e-012 4.079e-012 -11.355 -11.389 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.77 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.86 -3.69 -2.84 O2

Initial solution 100. 30/8/2012 12:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.114e-004 4.114e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.608e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.143e-003

Total CO2 (mol/kg) = 4.143e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.02

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551902e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9897 0.8076

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.022e-007 9.434e-008 -6.991 -7.025 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.143e-003

HCO3- 3.585e-003 3.320e-003 -2.446 -2.479 -0.033

CO2 4.987e-004 4.994e-004 -3.302 -3.302 0.001

CaHCO3+ 3.783e-005 3.504e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

CaCO3 3.069e-006 3.073e-006 -5.513 -5.512 0.001

CO3-2 2.994e-006 2.204e-006 -5.524 -5.657 -0.133

MgCO3 6.907e-007 6.916e-007 -6.161 -6.160 0.001

NaHCO3 1.722e-008 1.725e-008 -7.764 -7.763 0.001

NaCO3- 2.826e-010 2.612e-010 -9.549 -9.583 -0.034

Ca 1.332e-003

Ca+2 1.279e-003 9.404e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.783e-005 3.504e-005 -4.422 -4.455 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.069e-006 3.073e-006 -5.513 -5.512 0.001

CaOH+ 2.802e-009 2.590e-009 -8.552 -8.587 -0.034

CaHSO4+ 4.412e-012 4.078e-012 -11.355 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 5.526e-026

H2 2.763e-026 2.766e-026 -25.559 -25.558 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.471e-009 1.359e-009 -8.832 -8.867 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

MgSO4 5.099e-006 5.106e-006 -5.292 -5.292 0.001

MgCO3 6.907e-007 6.916e-007 -6.161 -6.160 0.001

MgOH+ 1.230e-008 1.137e-008 -7.910 -7.944 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.722e-008 1.725e-008 -7.764 -7.763 0.001

NaSO4- 3.427e-009 3.167e-009 -8.465 -8.499 -0.034

NaCO3- 2.826e-010 2.612e-010 -9.549 -9.583 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.114e-004

O2 2.057e-004 2.060e-004 -3.687 -3.686 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.099e-006 5.106e-006 -5.292 -5.292 0.001

NaSO4- 3.427e-009 3.167e-009 -8.465 -8.499 -0.034

KSO4- 1.471e-009 1.359e-009 -8.832 -8.867 -0.034

HSO4- 3.902e-010 3.607e-010 -9.409 -9.443 -0.034

CaHSO4+ 4.412e-012 4.078e-012 -11.355 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.85 -3.69 -2.84 O2

Initial solution 101. 30/8/2012 12:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.208e-004 4.208e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 297

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.143e-003

Total CO2 (mol/kg) = 4.143e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9821 0.8072

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.046e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.143e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.887e-004 4.893e-004 -3.311 -3.310 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CO3-2 3.073e-006 2.261e-006 -5.512 -5.646 -0.133

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.427e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

MgOH+ 1.258e-008 1.163e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.208e-004

O2 2.104e-004 2.107e-004 -3.677 -3.676 0.001

S(6) 1.154e-004

SO4-2 9.771e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

HSO4- 3.812e-010 3.523e-010 -9.419 -9.453 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.83 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.84 -3.68 -2.84 O2

Initial solution 102. 30/8/2012 13:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.201e-004 4.201e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.608e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.132e-003

Total CO2 (mol/kg) = 4.132e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.02

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551901e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9820 0.8071

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.046e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.322e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.132e-003

HCO3- 3.584e-003 3.320e-003 -2.446 -2.479 -0.033

CO2 4.873e-004 4.880e-004 -3.312 -3.312 0.001

CaHCO3+ 3.783e-005 3.504e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

CaCO3 3.140e-006 3.144e-006 -5.503 -5.502 0.001

CO3-2 3.064e-006 2.255e-006 -5.514 -5.647 -0.133

MgCO3 7.067e-007 7.077e-007 -6.151 -6.150 0.001

NaHCO3 1.722e-008 1.724e-008 -7.764 -7.763 0.001

NaCO3- 2.892e-010 2.673e-010 -9.539 -9.573 -0.034

Ca 1.332e-003

Ca+2 1.278e-003 9.404e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.783e-005 3.504e-005 -4.422 -4.455 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.140e-006 3.144e-006 -5.503 -5.502 0.001

CaOH+ 2.867e-009 2.650e-009 -8.543 -8.577 -0.034

CaHSO4+ 4.311e-012 3.985e-012 -11.365 -11.400 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.471e-009 1.359e-009 -8.832 -8.867 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

MgSO4 5.099e-006 5.106e-006 -5.292 -5.292 0.001

MgCO3 7.067e-007 7.077e-007 -6.151 -6.150 0.001

MgOH+ 1.259e-008 1.163e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.722e-008 1.724e-008 -7.764 -7.763 0.001

NaSO4- 3.427e-009 3.167e-009 -8.465 -8.499 -0.034

NaCO3- 2.892e-010 2.673e-010 -9.539 -9.573 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.201e-004

O2 2.101e-004 2.103e-004 -3.678 -3.677 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.170e-005 -4.010 -4.145 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.099e-006 5.106e-006 -5.292 -5.292 0.001

NaSO4- 3.427e-009 3.167e-009 -8.465 -8.499 -0.034

KSO4- 1.471e-009 1.359e-009 -8.832 -8.867 -0.034

HSO4- 3.813e-010 3.525e-010 -9.419 -9.453 -0.034

CaHSO4+ 4.311e-012 3.985e-012 -11.365 -11.400 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.76 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.84 -3.68 -2.84 O2

Initial solution 103. 30/8/2012 13:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.932e-004 3.932e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.144e-003

Total CO2 (mol/kg) = 4.144e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551901e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9835 0.8070

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.037e-007 9.575e-008 -6.984 -7.019 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.144e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.895e-004 4.902e-004 -3.310 -3.310 0.001

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CO3-2 3.066e-006 2.256e-006 -5.513 -5.647 -0.133

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.282e-026

H2 2.641e-026 2.645e-026 -25.578 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

MgOH+ 1.247e-008 1.152e-008 -7.904 -7.939 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.932e-004

O2 1.966e-004 1.969e-004 -3.706 -3.706 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.805e-010 3.516e-010 -9.420 -9.454 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.87 -3.71 -2.84 O2

Initial solution 104. 30/8/2012 13:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.239e-004 4.239e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 297

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.143e-003

Total CO2 (mol/kg) = 4.143e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9829 0.8072

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.046e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.143e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.887e-004 4.893e-004 -3.311 -3.310 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CO3-2 3.073e-006 2.261e-006 -5.512 -5.646 -0.133

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.427e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

MgOH+ 1.258e-008 1.163e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.239e-004

O2 2.119e-004 2.122e-004 -3.674 -3.673 0.001

S(6) 1.154e-004

SO4-2 9.771e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

HSO4- 3.812e-010 3.523e-010 -9.419 -9.453 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.83 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.84 -3.67 -2.84 O2

Initial solution 105. 30/8/2012 13:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.951e-004 3.951e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 297

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.132e-003

Total CO2 (mol/kg) = 4.132e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551899e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9653 0.8062

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.070e-007 9.878e-008 -6.971 -7.005 -0.035

H+ 6.179e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.132e-003

HCO3- 3.594e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.775e-004 4.781e-004 -3.321 -3.320 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.230e-006 3.234e-006 -5.491 -5.490 0.001

CO3-2 3.144e-006 2.313e-006 -5.502 -5.636 -0.133

MgCO3 7.249e-007 7.258e-007 -6.140 -6.139 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.967e-010 2.742e-010 -9.528 -9.562 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.426e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.230e-006 3.234e-006 -5.491 -5.490 0.001

CaOH+ 2.941e-009 2.718e-009 -8.531 -8.566 -0.034

CaHSO4+ 4.222e-012 3.902e-012 -11.375 -11.409 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.039e-026

H2 2.520e-026 2.523e-026 -25.599 -25.598 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

MgCO3 7.249e-007 7.258e-007 -6.140 -6.139 0.001

MgOH+ 1.288e-008 1.190e-008 -7.890 -7.924 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

NaCO3- 2.967e-010 2.742e-010 -9.528 -9.562 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 3.951e-004

O2 1.976e-004 1.978e-004 -3.704 -3.704 0.001

S(6) 1.154e-004

SO4-2 9.771e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

HSO4- 3.725e-010 3.443e-010 -9.429 -9.463 -0.034

CaHSO4+ 4.222e-012 3.902e-012 -11.375 -11.409 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.38 CO2

Dolomite -0.81 -17.73 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.87 -3.70 -2.84 O2

Initial solution 106. 30/8/2012 14:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.039e-004 4.039e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 297

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.143e-003

Total CO2 (mol/kg) = 4.143e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551902e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9777 0.8069

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.046e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.143e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.887e-004 4.893e-004 -3.311 -3.310 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CO3-2 3.073e-006 2.261e-006 -5.512 -5.646 -0.133

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.427e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

MgOH+ 1.258e-008 1.163e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.039e-004

O2 2.019e-004 2.022e-004 -3.695 -3.694 0.001

S(6) 1.154e-004

SO4-2 9.771e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

HSO4- 3.812e-010 3.523e-010 -9.419 -9.453 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.83 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.86 -3.69 -2.84 O2

Initial solution 107. 30/8/2012 14:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.982e-004 3.982e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 297

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.132e-003

Total CO2 (mol/kg) = 4.132e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551900e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9662 0.8062

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.070e-007 9.878e-008 -6.971 -7.005 -0.035

H+ 6.179e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.132e-003

HCO3- 3.594e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.775e-004 4.781e-004 -3.321 -3.320 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.230e-006 3.234e-006 -5.491 -5.490 0.001

CO3-2 3.144e-006 2.313e-006 -5.502 -5.636 -0.133

MgCO3 7.249e-007 7.258e-007 -6.140 -6.139 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.967e-010 2.742e-010 -9.528 -9.562 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.426e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.230e-006 3.234e-006 -5.491 -5.490 0.001

CaOH+ 2.941e-009 2.718e-009 -8.531 -8.566 -0.034

CaHSO4+ 4.222e-012 3.902e-012 -11.375 -11.409 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.039e-026

H2 2.520e-026 2.523e-026 -25.599 -25.598 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

MgCO3 7.249e-007 7.258e-007 -6.140 -6.139 0.001

MgOH+ 1.288e-008 1.190e-008 -7.890 -7.924 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

NaCO3- 2.967e-010 2.742e-010 -9.528 -9.562 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 3.982e-004

O2 1.991e-004 1.994e-004 -3.701 -3.700 0.001

S(6) 1.154e-004

SO4-2 9.771e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

HSO4- 3.725e-010 3.443e-010 -9.429 -9.463 -0.034

CaHSO4+ 4.222e-012 3.902e-012 -11.375 -11.409 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.38 CO2

Dolomite -0.81 -17.73 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.86 -3.70 -2.84 O2

Initial solution 108. 30/8/2012 14:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.801e-004 3.801e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 297

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.143e-003

Total CO2 (mol/kg) = 4.143e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551900e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9711 0.8065

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.046e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.143e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.887e-004 4.893e-004 -3.311 -3.310 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CO3-2 3.073e-006 2.261e-006 -5.512 -5.646 -0.133

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.427e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

MgOH+ 1.258e-008 1.163e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.801e-004

O2 1.901e-004 1.903e-004 -3.721 -3.721 0.001

S(6) 1.154e-004

SO4-2 9.771e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

HSO4- 3.812e-010 3.523e-010 -9.419 -9.453 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.83 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.88 -3.72 -2.84 O2

Initial solution 109. 30/8/2012 15:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.045e-004 4.045e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 298

Density (g/cm3) = 0.99887

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.142e-003

Total CO2 (mol/kg) = 4.142e-003

Temperature (deg C) = 17.900

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551902e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9692 0.8067

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.054e-007 9.732e-008 -6.977 -7.012 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.142e-003

HCO3- 3.594e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.879e-004 4.885e-004 -3.312 -3.311 0.001

CaHCO3+ 3.810e-005 3.529e-005 -4.419 -4.452 -0.033

MgHCO3+ 1.508e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.168e-006 3.173e-006 -5.499 -5.499 0.001

CO3-2 3.080e-006 2.266e-006 -5.511 -5.645 -0.133

MgCO3 7.112e-007 7.121e-007 -6.148 -6.147 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.922e-010 2.701e-010 -9.534 -9.569 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.426e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.810e-005 3.529e-005 -4.419 -4.452 -0.033

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

CaCO3 3.168e-006 3.173e-006 -5.499 -5.499 0.001

CaOH+ 2.874e-009 2.656e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.328e-012 3.999e-012 -11.364 -11.398 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.271e-026

H2 2.636e-026 2.639e-026 -25.579 -25.579 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.473e-009 1.361e-009 -8.832 -8.866 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.508e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.107e-006 5.114e-006 -5.292 -5.291 0.001

MgCO3 7.112e-007 7.121e-007 -6.148 -6.147 0.001

MgOH+ 1.270e-008 1.174e-008 -7.896 -7.930 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.427e-009 3.167e-009 -8.465 -8.499 -0.034

NaCO3- 2.922e-010 2.701e-010 -9.534 -9.569 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.045e-004

O2 2.023e-004 2.025e-004 -3.694 -3.694 0.001

S(6) 1.154e-004

SO4-2 9.769e-005 7.164e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

MgSO4 5.107e-006 5.114e-006 -5.292 -5.291 0.001

NaSO4- 3.427e-009 3.167e-009 -8.465 -8.499 -0.034

KSO4- 1.473e-009 1.361e-009 -8.832 -8.866 -0.034

HSO4- 3.819e-010 3.529e-010 -9.418 -9.452 -0.034

CaHSO4+ 4.328e-012 3.999e-012 -11.364 -11.398 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.83 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.86 -3.69 -2.84 O2

Initial solution 110. 30/8/2012 15:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.620e-003 3.620e-003

Ca 1.321e-003 1.321e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.645e-004 3.645e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 294

Density (g/cm3) = 0.99888

Activity of water = 1.000

Ionic strength = 5.572e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.097e-003

Total CO2 (mol/kg) = 4.097e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.165e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.92

Iterations = 7

Total H = 1.110160e+002

Total O = 5.551885e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9666 0.8063

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.045e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.321e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.097e-003

HCO3- 3.554e-003 3.293e-003 -2.449 -2.482 -0.033

CO2 4.834e-004 4.840e-004 -3.316 -3.315 0.001

CaHCO3+ 3.723e-005 3.449e-005 -4.429 -4.462 -0.033

MgHCO3+ 1.493e-005 1.380e-005 -4.826 -4.860 -0.034

CaCO3 3.092e-006 3.096e-006 -5.510 -5.509 0.001

CO3-2 3.036e-006 2.236e-006 -5.518 -5.650 -0.133

MgCO3 7.017e-007 7.026e-007 -6.154 -6.153 0.001

NaHCO3 1.708e-008 1.711e-008 -7.767 -7.767 0.001

NaCO3- 2.868e-010 2.652e-010 -9.542 -9.576 -0.034

Ca 1.321e-003

Ca+2 1.268e-003 9.335e-004 -2.897 -3.030 -0.133

CaHCO3+ 3.723e-005 3.449e-005 -4.429 -4.462 -0.033

CaSO4 1.247e-005 1.248e-005 -4.904 -4.904 0.001

CaCO3 3.092e-006 3.096e-006 -5.510 -5.509 0.001

CaOH+ 2.846e-009 2.631e-009 -8.546 -8.580 -0.034

CaHSO4+ 4.285e-012 3.961e-012 -11.368 -11.402 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.290e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.070e-006 -5.478 -5.513 -0.035

KSO4- 1.473e-009 1.362e-009 -8.832 -8.866 -0.034

KOH 1.805e-013 1.808e-013 -12.743 -12.743 0.001

Mg 5.184e-004

Mg+2 4.977e-004 3.678e-004 -3.303 -3.434 -0.131

MgHCO3+ 1.493e-005 1.380e-005 -4.826 -4.860 -0.034

MgSO4 5.112e-006 5.119e-006 -5.291 -5.291 0.001

MgCO3 7.017e-007 7.026e-007 -6.154 -6.153 0.001

MgOH+ 1.260e-008 1.165e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.239e-006 -5.001 -5.034 -0.034

NaHCO3 1.708e-008 1.711e-008 -7.767 -7.767 0.001

NaSO4- 3.432e-009 3.173e-009 -8.464 -8.499 -0.034

NaCO3- 2.868e-010 2.652e-010 -9.542 -9.576 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.984 0.001

O(0) 3.645e-004

O2 1.822e-004 1.825e-004 -3.739 -3.739 0.001

S(6) 1.154e-004

SO4-2 9.779e-005 7.180e-005 -4.010 -4.144 -0.134

CaSO4 1.247e-005 1.248e-005 -4.904 -4.904 0.001

MgSO4 5.112e-006 5.119e-006 -5.291 -5.291 0.001

NaSO4- 3.432e-009 3.173e-009 -8.464 -8.499 -0.034

KSO4- 1.473e-009 1.362e-009 -8.832 -8.866 -0.034

HSO4- 3.818e-010 3.530e-010 -9.418 -9.452 -0.034

CaHSO4+ 4.285e-012 3.961e-012 -11.368 -11.402 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.38 CO2

Dolomite -0.85 -17.77 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.90 -3.74 -2.84 O2

Initial solution 111. 30/8/2012 15:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.839e-004 3.839e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 297

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.143e-003

Total CO2 (mol/kg) = 4.143e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551900e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9722 0.8066

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.046e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.143e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.887e-004 4.893e-004 -3.311 -3.310 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CO3-2 3.073e-006 2.261e-006 -5.512 -5.646 -0.133

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.427e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

MgOH+ 1.258e-008 1.163e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.839e-004

O2 1.919e-004 1.922e-004 -3.717 -3.716 0.001

S(6) 1.154e-004

SO4-2 9.771e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

HSO4- 3.812e-010 3.523e-010 -9.419 -9.453 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.83 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.88 -3.72 -2.84 O2

Initial solution 112. 30/8/2012 15:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.631e-003 3.631e-003

Ca 1.325e-003 1.325e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.939e-004 3.939e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99888

Activity of water = 1.000

Ionic strength = 5.584e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.108e-003

Total CO2 (mol/kg) = 4.108e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.195e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.95

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551891e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9750 0.8067

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.046e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.322e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.108e-003

HCO3- 3.564e-003 3.302e-003 -2.448 -2.481 -0.033

CO2 4.847e-004 4.853e-004 -3.315 -3.314 0.001

CaHCO3+ 3.743e-005 3.468e-005 -4.427 -4.460 -0.033

MgHCO3+ 1.496e-005 1.383e-005 -4.825 -4.859 -0.034

CaCO3 3.108e-006 3.112e-006 -5.508 -5.507 0.001

CO3-2 3.045e-006 2.242e-006 -5.516 -5.649 -0.133

MgCO3 7.034e-007 7.043e-007 -6.153 -6.152 0.001

NaHCO3 1.713e-008 1.715e-008 -7.766 -7.766 0.001

NaCO3- 2.876e-010 2.659e-010 -9.541 -9.575 -0.034

Ca 1.325e-003

Ca+2 1.271e-003 9.358e-004 -2.896 -3.029 -0.133

CaHCO3+ 3.743e-005 3.468e-005 -4.427 -4.460 -0.033

CaSO4 1.249e-005 1.251e-005 -4.903 -4.903 0.001

CaCO3 3.108e-006 3.112e-006 -5.508 -5.507 0.001

CaOH+ 2.853e-009 2.637e-009 -8.545 -8.579 -0.034

CaHSO4+ 4.294e-012 3.969e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.070e-006 -5.478 -5.513 -0.035

KSO4- 1.472e-009 1.361e-009 -8.832 -8.866 -0.034

KOH 1.805e-013 1.807e-013 -12.743 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.676e-004 -3.303 -3.435 -0.131

MgHCO3+ 1.496e-005 1.383e-005 -4.825 -4.859 -0.034

MgSO4 5.108e-006 5.115e-006 -5.292 -5.291 0.001

MgCO3 7.034e-007 7.043e-007 -6.153 -6.152 0.001

MgOH+ 1.259e-008 1.164e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.238e-006 -5.001 -5.034 -0.034

NaHCO3 1.713e-008 1.715e-008 -7.766 -7.766 0.001

NaSO4- 3.430e-009 3.171e-009 -8.465 -8.499 -0.034

NaCO3- 2.876e-010 2.659e-010 -9.541 -9.575 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.984 0.001

O(0) 3.939e-004

O2 1.969e-004 1.972e-004 -3.706 -3.705 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.177e-005 -4.010 -4.144 -0.134

CaSO4 1.249e-005 1.251e-005 -4.903 -4.903 0.001

MgSO4 5.108e-006 5.115e-006 -5.292 -5.291 0.001

NaSO4- 3.430e-009 3.171e-009 -8.465 -8.499 -0.034

KSO4- 1.472e-009 1.361e-009 -8.832 -8.866 -0.034

HSO4- 3.817e-010 3.528e-010 -9.418 -9.452 -0.034

CaHSO4+ 4.294e-012 3.969e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.94 -3.31 -1.38 CO2

Dolomite -0.84 -17.76 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.87 -3.71 -2.84 O2

Initial solution 113. 30/8/2012 16:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.957e-004 3.957e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.144e-003

Total CO2 (mol/kg) = 4.144e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551902e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9842 0.8070

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.037e-007 9.575e-008 -6.984 -7.019 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.144e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.895e-004 4.902e-004 -3.310 -3.310 0.001

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CO3-2 3.066e-006 2.256e-006 -5.513 -5.647 -0.133

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.282e-026

H2 2.641e-026 2.645e-026 -25.578 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

MgOH+ 1.247e-008 1.152e-008 -7.904 -7.939 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.957e-004

O2 1.979e-004 1.981e-004 -3.704 -3.703 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.805e-010 3.516e-010 -9.420 -9.454 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.87 -3.70 -2.84 O2

Initial solution 114. 30/8/2012 16:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.670e-004 3.670e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.144e-003

Total CO2 (mol/kg) = 4.144e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551899e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9760 0.8065

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.037e-007 9.575e-008 -6.984 -7.019 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.144e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.895e-004 4.902e-004 -3.310 -3.310 0.001

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CO3-2 3.066e-006 2.256e-006 -5.513 -5.647 -0.133

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.282e-026

H2 2.641e-026 2.645e-026 -25.578 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

MgOH+ 1.247e-008 1.152e-008 -7.904 -7.939 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.670e-004

O2 1.835e-004 1.837e-004 -3.736 -3.736 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.805e-010 3.516e-010 -9.420 -9.454 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.90 -3.74 -2.84 O2

Initial solution 115. 30/8/2012 16:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.945e-004 3.945e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.144e-003

Total CO2 (mol/kg) = 4.144e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551902e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9839 0.8070

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.037e-007 9.575e-008 -6.984 -7.019 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.144e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.895e-004 4.902e-004 -3.310 -3.310 0.001

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CO3-2 3.066e-006 2.256e-006 -5.513 -5.647 -0.133

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.282e-026

H2 2.641e-026 2.645e-026 -25.578 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

MgOH+ 1.247e-008 1.152e-008 -7.904 -7.939 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.945e-004

O2 1.972e-004 1.975e-004 -3.705 -3.704 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.805e-010 3.516e-010 -9.420 -9.454 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.87 -3.70 -2.84 O2

Initial solution 116. 30/8/2012 16:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.976e-004 3.976e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.168e-003

Total CO2 (mol/kg) = 4.168e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551908e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0034 0.8078

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.005e-007 9.281e-008 -6.998 -7.032 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.168e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.032e-004 5.039e-004 -3.298 -3.298 0.001

CaHCO3+ 3.809e-005 3.527e-005 -4.419 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.078e-006 3.082e-006 -5.512 -5.511 0.001

CO3-2 2.998e-006 2.205e-006 -5.523 -5.657 -0.133

MgCO3 6.887e-007 6.896e-007 -6.162 -6.161 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.799e-010 2.586e-010 -9.553 -9.587 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.452e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.809e-005 3.527e-005 -4.419 -4.453 -0.033

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

CaCO3 3.078e-006 3.082e-006 -5.512 -5.511 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.585 -0.034

CaHSO4+ 4.415e-012 4.080e-012 -11.355 -11.389 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.537e-026

H2 2.769e-026 2.772e-026 -25.558 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.465e-009 1.354e-009 -8.834 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.066e-006 5.073e-006 -5.295 -5.295 0.001

MgCO3 6.887e-007 6.896e-007 -6.162 -6.161 0.001

MgOH+ 1.206e-008 1.115e-008 -7.918 -7.953 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.799e-010 2.586e-010 -9.553 -9.587 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.976e-004

O2 1.988e-004 1.991e-004 -3.702 -3.701 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

MgSO4 5.066e-006 5.073e-006 -5.295 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.465e-009 1.354e-009 -8.834 -8.869 -0.034

HSO4- 3.885e-010 3.590e-010 -9.411 -9.445 -0.034

CaHSO4+ 4.415e-012 4.080e-012 -11.355 -11.389 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.70 -2.83 O2

Initial solution 117. 30/8/2012 17:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.014e-004 4.014e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551910e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0244 0.8090

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.601e-008 8.863e-008 -7.018 -7.052 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.596e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.256e-004 5.263e-004 -3.279 -3.279 0.001

CaHCO3+ 3.790e-005 3.510e-005 -4.421 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 2.926e-006 2.929e-006 -5.534 -5.533 0.001

CO3-2 2.855e-006 2.101e-006 -5.544 -5.678 -0.133

MgCO3 6.563e-007 6.572e-007 -6.183 -6.182 0.001

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaCO3- 2.666e-010 2.464e-010 -9.574 -9.608 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.790e-005 3.510e-005 -4.421 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 2.926e-006 2.929e-006 -5.534 -5.533 0.001

CaOH+ 2.684e-009 2.480e-009 -8.571 -8.606 -0.034

CaHSO4+ 4.614e-012 4.264e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.071e-026

H2 3.036e-026 3.040e-026 -25.518 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.465e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.563e-007 6.572e-007 -6.183 -6.182 0.001

MgOH+ 1.153e-008 1.065e-008 -7.938 -7.973 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.666e-010 2.464e-010 -9.574 -9.608 -0.034

NaOH 9.658e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 4.014e-004

O2 2.007e-004 2.009e-004 -3.697 -3.697 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.465e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 4.070e-010 3.761e-010 -9.390 -9.425 -0.034

CaHSO4+ 4.614e-012 4.264e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.38 CO2

Dolomite -0.90 -17.82 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 118. 30/8/2012 17:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.083e-004 4.083e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.157e-003

Total CO2 (mol/kg) = 4.157e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0063 0.8080

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.005e-007 9.281e-008 -6.998 -7.032 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.157e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.019e-004 5.025e-004 -3.299 -3.299 0.001

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CO3-2 2.989e-006 2.199e-006 -5.524 -5.658 -0.133

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.537e-026

H2 2.769e-026 2.772e-026 -25.558 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

MgOH+ 1.207e-008 1.115e-008 -7.918 -7.953 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.083e-004

O2 2.041e-004 2.044e-004 -3.690 -3.690 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.886e-010 3.592e-010 -9.410 -9.445 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.69 -2.83 O2

Initial solution 119. 30/8/2012 17:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.995e-004 3.995e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.157e-003

Total CO2 (mol/kg) = 4.157e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0039 0.8079

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.005e-007 9.281e-008 -6.998 -7.032 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.157e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.019e-004 5.025e-004 -3.299 -3.299 0.001

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CO3-2 2.989e-006 2.199e-006 -5.524 -5.658 -0.133

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.537e-026

H2 2.769e-026 2.772e-026 -25.558 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

MgOH+ 1.207e-008 1.115e-008 -7.918 -7.953 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.995e-004

O2 1.997e-004 2.000e-004 -3.700 -3.699 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.886e-010 3.592e-010 -9.410 -9.445 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 120. 30/8/2012 17:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.857e-004 3.857e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.192e-003

Total CO2 (mol/kg) = 4.192e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0201 0.8088

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.602e-008 8.863e-008 -7.018 -7.052 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.192e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.270e-004 5.277e-004 -3.278 -3.278 0.001

CaHCO3+ 3.809e-005 3.528e-005 -4.419 -4.452 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.941e-006 2.944e-006 -5.532 -5.531 0.001

CO3-2 2.863e-006 2.106e-006 -5.543 -5.676 -0.133

MgCO3 6.579e-007 6.587e-007 -6.182 -6.181 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.673e-010 2.470e-010 -9.573 -9.607 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.453e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.809e-005 3.528e-005 -4.419 -4.452 -0.033

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

CaCO3 2.941e-006 2.944e-006 -5.532 -5.531 0.001

CaOH+ 2.690e-009 2.486e-009 -8.570 -8.604 -0.034

CaHSO4+ 4.623e-012 4.272e-012 -11.335 -11.369 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.071e-026

H2 3.036e-026 3.040e-026 -25.518 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.465e-009 1.354e-009 -8.834 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.066e-006 5.073e-006 -5.295 -5.295 0.001

MgCO3 6.579e-007 6.587e-007 -6.182 -6.181 0.001

MgOH+ 1.152e-008 1.065e-008 -7.938 -7.973 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.420e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.673e-010 2.470e-010 -9.573 -9.607 -0.034

NaOH 9.657e-013 9.669e-013 -12.015 -12.015 0.001

O(0) 3.857e-004

O2 1.929e-004 1.931e-004 -3.715 -3.714 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

MgSO4 5.066e-006 5.073e-006 -5.295 -5.295 0.001

NaSO4- 3.420e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.465e-009 1.354e-009 -8.834 -8.869 -0.034

HSO4- 4.068e-010 3.759e-010 -9.391 -9.425 -0.034

CaHSO4+ 4.623e-012 4.272e-012 -11.335 -11.369 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.38 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

------------------

End of simulation.

------------------

------------------------------------

Reading input data for simulation 2.

------------------------------------

-----------

End of run.

-----------

**D.2. Maolan**

Input file: C:\Users\huan\Desktop\Maolan Spring.pqi

Output file: C:\Users\huan\Desktop\Maolan Spring.pqo

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

------------------

Reading data base.

------------------

SOLUTION\_MASTER\_SPECIES

SOLUTION\_SPECIES

PHASES

EXCHANGE\_MASTER\_SPECIES

EXCHANGE\_SPECIES

SURFACE\_MASTER\_SPECIES

SURFACE\_SPECIES

RATES

END

------------------------------------

Reading input data for simulation 1.

------------------------------------

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

SOLUTION\_SPREAD

units mg/l

Description Number pH Temp O(0) Ca K Mg Na S(6) Cl Alkalinity

mg/L mg/L mg/L mg/L mg/L mg/L mg/L mg/L as HCO3

29/8/2012 11:54:20 1 7.28 17.7 6.68 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

29/8/2012 12:09:20 2 7.23 17.8 6.34 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

29/8/2012 12:24:20 3 7.24 17.7 6.8 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

29/8/2012 12:39:20 4 7.23 17.7 6.8 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

29/8/2012 12:54:20 5 7.22 17.7 6.7 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

29/8/2012 13:09:20 6 7.23 17.7 6.63 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

29/8/2012 13:24:20 7 7.2 17.7 6.46 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

29/8/2012 13:39:20 8 7.16 17.7 6.55 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

29/8/2012 13:54:20 9 7.22 17.6 6.73 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

29/8/2012 14:09:20 10 7.22 17.6 6.44 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

29/8/2012 14:24:20 11 7.21 17.6 6.54 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

29/8/2012 14:39:20 12 7.22 17.6 6.7 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

29/8/2012 14:54:20 13 7.2 17.6 6.63 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

29/8/2012 15:09:20 14 7.2 17.6 6.42 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 15:24:20 15 7.21 17.5 6.37 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 15:39:20 16 7.16 17.5 6.45 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 15:54:20 17 7.2 17.5 6.3 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 16:09:20 18 7.2 17.5 6.21 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 16:24:20 19 7.16 17.5 6.2 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 16:39:20 20 7.2 17.5 6 53.82 0.13 12.60 0.23 11.07999992 2.029999971 224.61

29/8/2012 16:54:20 21 7.19 17.5 6.04 53.82 0.13 12.60 0.23 11.07999992 2.029999971 224.61

29/8/2012 17:09:20 22 7.21 17.5 5.91 53.82 0.13 12.60 0.23 11.07999992 2.029999971 224.61

29/8/2012 17:24:20 23 7.22 17.5 6.09 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 17:39:20 24 7.2 17.5 6.41 53.82 0.13 12.60 0.23 11.07999992 2.029999971 224.61

29/8/2012 17:54:20 25 7.22 17.5 6.12 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 18:09:20 26 7.21 17.5 6.24 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 18:24:20 27 7.2 17.5 6.1 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 18:39:20 28 7.19 17.5 6 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 18:54:20 29 7.2 17.5 6.19 53.82 0.13 12.60 0.23 11.07999992 2.029999971 224.61

29/8/2012 19:09:20 30 7.22 17.5 6.34 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 19:24:20 31 7.2 17.5 6.12 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 19:39:20 32 7.11 17.5 6.23 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 19:54:20 33 7.19 17.5 6.7 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 20:09:20 34 7.21 17.5 6.08 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 20:24:20 35 7.2 17.5 6.58 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 20:39:20 36 7.19 17.5 6.16 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 20:54:20 37 7.19 17.5 6.25 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 21:09:20 38 7.19 17.5 6.4 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 21:24:20 39 7.27 17.5 6.67 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 21:39:20 40 7.19 17.5 6.06 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 21:54:20 41 7.16 17.5 6.01 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 22:09:20 42 7.2 17.5 5.99 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 22:24:20 43 7.24 17.4 6.47 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 22:39:20 44 7.13 17.5 6.08 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 22:54:20 45 7.22 17.5 6.03 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 23:09:20 46 7.22 17.4 6.04 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 23:24:20 47 7.22 17.5 6.56 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 23:39:20 48 7.21 17.4 6.79 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

29/8/2012 23:54:20 49 7.22 17.5 6.44 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 00:09:20 50 7.21 17.4 7.05 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 00:24:20 51 7.21 17.5 5.93 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 00:39:20 52 7.21 17.5 5.94 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 00:54:20 53 7.21 17.4 6.74 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 01:09:20 54 7.22 17.5 6.31 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 01:24:20 55 7.21 17.5 6.05 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 01:39:20 56 7.22 17.5 6.62 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 01:54:20 57 7.21 17.5 6.17 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 02:09:20 58 7.22 17.5 5.94 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 02:24:20 59 7.22 17.4 6.75 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 02:39:20 60 7.21 17.5 6.79 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 02:54:20 61 7.22 17.4 6.11 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 03:09:20 62 7.22 17.4 6.12 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 03:24:20 63 7.22 17.5 6.54 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 03:39:20 64 7.14 17.5 6.1 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 03:54:20 65 7.22 17.5 6.47 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 04:09:20 66 7.22 17.5 6.5 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 04:24:20 67 7.22 17.5 6.83 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 04:39:20 68 7.22 17.5 6.9 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 04:54:20 69 7.23 17.5 6.41 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 05:09:20 70 7.17 17.5 6.19 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 05:24:20 71 7.2 17.5 6.43 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 05:39:20 72 7.16 17.5 6.41 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 05:54:20 73 7.25 17.5 6.43 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 06:09:20 74 7.24 17.5 6.7 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 06:24:20 75 7.22 17.5 6.33 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 06:39:20 76 7.24 17.5 6.64 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 06:54:20 77 7.2 17.5 5.91 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 07:09:20 78 7.21 17.5 6.13 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 07:24:20 79 7.22 17.5 6.37 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 07:39:20 80 7.23 17.5 6.21 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 07:54:20 81 7.24 17.5 5.84 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 08:09:20 82 7.23 17.5 6.3 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 08:24:20 83 7.24 17.5 6.18 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 08:39:20 84 7.24 17.5 5.96 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 08:54:20 85 7.23 17.5 5.94 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 09:09:20 86 7.23 17.5 6.63 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 09:24:20 87 7.23 17.5 6.64 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 09:39:20 88 7.23 17.5 6.44 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 09:54:20 89 7.23 17.5 6.13 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 10:09:20 90 7.23 17.5 5.79 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 10:24:20 91 7.23 17.5 6.4 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 10:39:20 92 7.23 17.5 6.04 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 10:54:20 93 7.23 17.6 6.05 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 11:09:20 94 7.22 17.6 6.23 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 11:24:20 95 7.22 17.7 6.24 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 11:39:20 96 7.22 17.6 6.45 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 11:54:20 97 7.22 17.7 6.36 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 12:09:20 98 7.22 17.7 6.11 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 12:24:20 99 7.22 17.7 6.49 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 12:39:20 100 7.22 17.8 6.58 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

30/8/2012 12:54:20 101 7.23 17.8 6.73 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 13:09:20 102 7.23 17.8 6.72 53.37 0.13 12.60 0.23 11.07999992 2.029999971 222.72

30/8/2012 13:24:20 103 7.23 17.7 6.29 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 13:39:20 104 7.23 17.8 6.78 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 13:54:20 105 7.24 17.8 6.32 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 14:09:20 106 7.23 17.8 6.46 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 14:24:20 107 7.24 17.8 6.37 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 14:54:20 108 7.23 17.8 6.08 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 15:09:20 109 7.23 17.9 6.47 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 15:24:20 110 7.23 17.8 5.83 52.92 0.13 12.60 0.23 11.07999992 2.029999971 220.83

30/8/2012 15:39:20 111 7.23 17.8 6.14 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 15:54:20 112 7.23 17.8 6.3 53.07 0.13 12.60 0.23 11.07999992 2.029999971 221.47

30/8/2012 16:09:20 113 7.23 17.7 6.33 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 16:24:20 114 7.23 17.7 5.87 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 16:39:20 115 7.23 17.7 6.31 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 16:54:20 116 7.22 17.6 6.36 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

30/8/2012 17:09:20 117 7.2 17.6 6.42 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 17:24:20 118 7.22 17.6 6.53 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 17:39:20 119 7.22 17.6 6.39 53.52 0.13 12.60 0.23 11.07999992 2.029999971 223.36

30/8/2012 17:54:20 120 7.2 17.6 6.17 53.67 0.13 12.60 0.23 11.07999992 2.029999971 223.99

SELECTED\_OUTPUT

file C:\Users\huan\Desktop\selected output spring.sel

reset false

saturation\_indices Calcite CO2(g)

-------------------------------------------

Beginning of initial solution calculations.

-------------------------------------------

Initial solution 1. 29/8/2012 11:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.176e-004 4.176e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.280

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.607e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.078e-003

Total CO2 (mol/kg) = 4.078e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.02

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551890e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9400 0.8044

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.164e-007 1.074e-007 -6.934 -6.969 -0.035

H+ 5.635e-008 5.248e-008 -7.249 -7.280 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.078e-003

HCO3- 3.583e-003 3.319e-003 -2.446 -2.479 -0.033

CO2 4.349e-004 4.355e-004 -3.362 -3.361 0.001

CaHCO3+ 3.773e-005 3.494e-005 -4.423 -4.457 -0.033

MgHCO3+ 1.502e-005 1.389e-005 -4.823 -4.857 -0.034

CaCO3 3.508e-006 3.513e-006 -5.455 -5.454 0.001

CO3-2 3.428e-006 2.523e-006 -5.465 -5.598 -0.133

MgCO3 7.895e-007 7.905e-007 -6.103 -6.102 0.001

NaHCO3 1.721e-008 1.724e-008 -7.764 -7.764 0.001

NaCO3- 3.219e-010 2.975e-010 -9.492 -9.527 -0.034

Ca 1.332e-003

Ca+2 1.278e-003 9.403e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.773e-005 3.494e-005 -4.423 -4.457 -0.033

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

CaCO3 3.508e-006 3.513e-006 -5.455 -5.454 0.001

CaOH+ 3.217e-009 2.973e-009 -8.493 -8.527 -0.034

CaHSO4+ 3.835e-012 3.545e-012 -11.416 -11.450 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 4.196e-026

H2 2.098e-026 2.101e-026 -25.678 -25.678 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

KOH 2.025e-013 2.028e-013 -12.694 -12.693 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.502e-005 1.389e-005 -4.823 -4.857 -0.034

MgSO4 5.087e-006 5.093e-006 -5.294 -5.293 0.001

MgCO3 7.895e-007 7.905e-007 -6.103 -6.102 0.001

MgOH+ 1.399e-008 1.293e-008 -7.854 -7.888 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.721e-008 1.724e-008 -7.764 -7.764 0.001

NaSO4- 3.426e-009 3.166e-009 -8.465 -8.499 -0.034

NaCO3- 3.219e-010 2.975e-010 -9.492 -9.527 -0.034

NaOH 1.161e-012 1.163e-012 -11.935 -11.935 0.001

O(0) 4.176e-004

O2 2.088e-004 2.091e-004 -3.680 -3.680 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.172e-005 -4.010 -4.144 -0.135

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

MgSO4 5.087e-006 5.093e-006 -5.294 -5.293 0.001

NaSO4- 3.426e-009 3.166e-009 -8.465 -8.499 -0.034

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

HSO4- 3.393e-010 3.136e-010 -9.469 -9.504 -0.034

CaHSO4+ 3.835e-012 3.545e-012 -11.416 -11.450 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.33 -8.62 -8.29 CaCO3

Calcite -0.18 -8.62 -8.44 CaCO3

CO2(g) -1.98 -3.36 -1.38 CO2

Dolomite -0.74 -17.66 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.56 -25.68 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.84 -3.68 -2.84 O2

Initial solution 2. 29/8/2012 12:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.964e-004 3.964e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.608e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.132e-003

Total CO2 (mol/kg) = 4.132e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.02

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551898e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9757 0.8068

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.046e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.322e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.132e-003

HCO3- 3.584e-003 3.320e-003 -2.446 -2.479 -0.033

CO2 4.873e-004 4.880e-004 -3.312 -3.312 0.001

CaHCO3+ 3.783e-005 3.504e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

CaCO3 3.140e-006 3.144e-006 -5.503 -5.502 0.001

CO3-2 3.064e-006 2.255e-006 -5.514 -5.647 -0.133

MgCO3 7.067e-007 7.077e-007 -6.151 -6.150 0.001

NaHCO3 1.722e-008 1.724e-008 -7.764 -7.763 0.001

NaCO3- 2.892e-010 2.673e-010 -9.539 -9.573 -0.034

Ca 1.332e-003

Ca+2 1.278e-003 9.404e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.783e-005 3.504e-005 -4.422 -4.455 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.140e-006 3.144e-006 -5.503 -5.502 0.001

CaOH+ 2.867e-009 2.650e-009 -8.543 -8.577 -0.034

CaHSO4+ 4.311e-012 3.985e-012 -11.365 -11.400 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.471e-009 1.359e-009 -8.832 -8.867 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

MgSO4 5.099e-006 5.106e-006 -5.292 -5.292 0.001

MgCO3 7.067e-007 7.077e-007 -6.151 -6.150 0.001

MgOH+ 1.259e-008 1.163e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.722e-008 1.724e-008 -7.764 -7.763 0.001

NaSO4- 3.427e-009 3.167e-009 -8.465 -8.499 -0.034

NaCO3- 2.892e-010 2.673e-010 -9.539 -9.573 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.964e-004

O2 1.982e-004 1.984e-004 -3.703 -3.702 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.170e-005 -4.010 -4.145 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.099e-006 5.106e-006 -5.292 -5.292 0.001

NaSO4- 3.427e-009 3.167e-009 -8.465 -8.499 -0.034

KSO4- 1.471e-009 1.359e-009 -8.832 -8.867 -0.034

HSO4- 3.813e-010 3.525e-010 -9.419 -9.453 -0.034

CaHSO4+ 4.311e-012 3.985e-012 -11.365 -11.400 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.76 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.87 -3.70 -2.84 O2

Initial solution 3. 29/8/2012 12:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.251e-004 4.251e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.608e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.121e-003

Total CO2 (mol/kg) = 4.121e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.02

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551899e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9820 0.8069

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.061e-007 9.798e-008 -6.974 -7.009 -0.035

H+ 6.178e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.121e-003

HCO3- 3.584e-003 3.320e-003 -2.446 -2.479 -0.033

CO2 4.770e-004 4.776e-004 -3.321 -3.321 0.001

CaHCO3+ 3.775e-005 3.496e-005 -4.423 -4.456 -0.033

MgHCO3+ 1.503e-005 1.389e-005 -4.823 -4.857 -0.034

CaCO3 3.201e-006 3.205e-006 -5.495 -5.494 0.001

CO3-2 3.127e-006 2.302e-006 -5.505 -5.638 -0.133

MgCO3 7.204e-007 7.213e-007 -6.142 -6.142 0.001

NaHCO3 1.722e-008 1.724e-008 -7.764 -7.763 0.001

NaCO3- 2.936e-010 2.714e-010 -9.532 -9.566 -0.034

Ca 1.332e-003

Ca+2 1.279e-003 9.404e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.775e-005 3.496e-005 -4.423 -4.456 -0.033

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

CaCO3 3.201e-006 3.205e-006 -5.495 -5.494 0.001

CaOH+ 2.934e-009 2.712e-009 -8.532 -8.567 -0.034

CaHSO4+ 4.206e-012 3.887e-012 -11.376 -11.410 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 5.045e-026

H2 2.522e-026 2.526e-026 -25.598 -25.598 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.503e-005 1.389e-005 -4.823 -4.857 -0.034

MgSO4 5.087e-006 5.094e-006 -5.294 -5.293 0.001

MgCO3 7.204e-007 7.213e-007 -6.142 -6.142 0.001

MgOH+ 1.276e-008 1.179e-008 -7.894 -7.928 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.722e-008 1.724e-008 -7.764 -7.763 0.001

NaSO4- 3.426e-009 3.166e-009 -8.465 -8.499 -0.034

NaCO3- 2.936e-010 2.714e-010 -9.532 -9.566 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 4.251e-004

O2 2.126e-004 2.128e-004 -3.673 -3.672 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

MgSO4 5.087e-006 5.094e-006 -5.294 -5.293 0.001

NaSO4- 3.426e-009 3.166e-009 -8.465 -8.499 -0.034

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

HSO4- 3.720e-010 3.438e-010 -9.429 -9.464 -0.034

CaHSO4+ 4.206e-012 3.887e-012 -11.376 -11.410 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.38 CO2

Dolomite -0.82 -17.74 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.84 -3.67 -2.84 O2

Initial solution 4. 29/8/2012 12:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.251e-004 4.251e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.608e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.132e-003

Total CO2 (mol/kg) = 4.132e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.02

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551901e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9920 0.8074

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.037e-007 9.575e-008 -6.984 -7.019 -0.035

H+ 6.322e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.132e-003

HCO3- 3.584e-003 3.320e-003 -2.446 -2.479 -0.033

CO2 4.882e-004 4.888e-004 -3.311 -3.311 0.001

CaHCO3+ 3.775e-005 3.497e-005 -4.423 -4.456 -0.033

MgHCO3+ 1.503e-005 1.389e-005 -4.823 -4.857 -0.034

CaCO3 3.129e-006 3.133e-006 -5.505 -5.504 0.001

CO3-2 3.056e-006 2.249e-006 -5.515 -5.648 -0.133

MgCO3 7.040e-007 7.050e-007 -6.152 -6.152 0.001

NaHCO3 1.722e-008 1.724e-008 -7.764 -7.763 0.001

NaCO3- 2.870e-010 2.652e-010 -9.542 -9.576 -0.034

Ca 1.332e-003

Ca+2 1.279e-003 9.405e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.775e-005 3.497e-005 -4.423 -4.456 -0.033

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

CaCO3 3.129e-006 3.133e-006 -5.505 -5.504 0.001

CaOH+ 2.868e-009 2.650e-009 -8.542 -8.577 -0.034

CaHSO4+ 4.304e-012 3.978e-012 -11.366 -11.400 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 5.282e-026

H2 2.641e-026 2.645e-026 -25.578 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.503e-005 1.389e-005 -4.823 -4.857 -0.034

MgSO4 5.087e-006 5.094e-006 -5.294 -5.293 0.001

MgCO3 7.040e-007 7.050e-007 -6.152 -6.152 0.001

MgOH+ 1.247e-008 1.152e-008 -7.904 -7.938 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.722e-008 1.724e-008 -7.764 -7.763 0.001

NaSO4- 3.425e-009 3.166e-009 -8.465 -8.499 -0.034

NaCO3- 2.870e-010 2.652e-010 -9.542 -9.576 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.251e-004

O2 2.126e-004 2.128e-004 -3.673 -3.672 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

MgSO4 5.087e-006 5.094e-006 -5.294 -5.293 0.001

NaSO4- 3.425e-009 3.166e-009 -8.465 -8.499 -0.034

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

HSO4- 3.807e-010 3.518e-010 -9.419 -9.454 -0.034

CaHSO4+ 4.304e-012 3.978e-012 -11.366 -11.400 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.76 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.84 -3.67 -2.84 O2

Initial solution 5. 29/8/2012 12:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.189e-004 4.189e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.608e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.144e-003

Total CO2 (mol/kg) = 4.144e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.01

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551903e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0004 0.8079

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.014e-007 9.357e-008 -6.994 -7.029 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.144e-003

HCO3- 3.585e-003 3.320e-003 -2.446 -2.479 -0.033

CO2 4.996e-004 5.002e-004 -3.301 -3.301 0.001

CaHCO3+ 3.776e-005 3.497e-005 -4.423 -4.456 -0.033

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

CaCO3 3.058e-006 3.062e-006 -5.515 -5.514 0.001

CO3-2 2.987e-006 2.198e-006 -5.525 -5.658 -0.133

MgCO3 6.881e-007 6.890e-007 -6.162 -6.162 0.001

NaHCO3 1.722e-008 1.725e-008 -7.764 -7.763 0.001

NaCO3- 2.805e-010 2.592e-010 -9.552 -9.586 -0.034

Ca 1.332e-003

Ca+2 1.279e-003 9.405e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.776e-005 3.497e-005 -4.423 -4.456 -0.033

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

CaCO3 3.058e-006 3.062e-006 -5.515 -5.514 0.001

CaOH+ 2.802e-009 2.590e-009 -8.552 -8.587 -0.034

CaHSO4+ 4.405e-012 4.071e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 5.531e-026

H2 2.766e-026 2.769e-026 -25.558 -25.558 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

MgSO4 5.087e-006 5.094e-006 -5.294 -5.293 0.001

MgCO3 6.881e-007 6.890e-007 -6.162 -6.162 0.001

MgOH+ 1.219e-008 1.126e-008 -7.914 -7.948 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.722e-008 1.725e-008 -7.764 -7.763 0.001

NaSO4- 3.425e-009 3.166e-009 -8.465 -8.499 -0.034

NaCO3- 2.805e-010 2.592e-010 -9.552 -9.586 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.189e-004

O2 2.094e-004 2.097e-004 -3.679 -3.678 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

MgSO4 5.087e-006 5.094e-006 -5.294 -5.293 0.001

NaSO4- 3.425e-009 3.166e-009 -8.465 -8.499 -0.034

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

HSO4- 3.895e-010 3.600e-010 -9.409 -9.444 -0.034

CaHSO4+ 4.405e-012 4.071e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.84 -3.68 -2.84 O2

Initial solution 6. 29/8/2012 13:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.145e-004 4.145e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.144e-003

Total CO2 (mol/kg) = 4.144e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9892 0.8073

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.037e-007 9.575e-008 -6.984 -7.019 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.144e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.895e-004 4.902e-004 -3.310 -3.310 0.001

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CO3-2 3.066e-006 2.256e-006 -5.513 -5.647 -0.133

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.282e-026

H2 2.641e-026 2.645e-026 -25.578 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

MgOH+ 1.247e-008 1.152e-008 -7.904 -7.939 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.145e-004

O2 2.073e-004 2.075e-004 -3.684 -3.683 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.805e-010 3.516e-010 -9.420 -9.454 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.85 -3.68 -2.84 O2

Initial solution 7. 29/8/2012 13:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.039e-004 4.039e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.608e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.168e-003

Total CO2 (mol/kg) = 4.168e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.01

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551906e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0164 0.8089

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.679e-008 8.936e-008 -7.014 -7.049 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.168e-003

HCO3- 3.585e-003 3.321e-003 -2.445 -2.479 -0.033

CO2 5.232e-004 5.239e-004 -3.281 -3.281 0.001

CaHCO3+ 3.777e-005 3.498e-005 -4.423 -4.456 -0.033

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

CaCO3 2.921e-006 2.925e-006 -5.534 -5.534 0.001

CO3-2 2.853e-006 2.100e-006 -5.545 -5.678 -0.133

MgCO3 6.573e-007 6.581e-007 -6.182 -6.182 0.001

NaHCO3 1.723e-008 1.725e-008 -7.764 -7.763 0.001

NaCO3- 2.679e-010 2.476e-010 -9.572 -9.606 -0.034

Ca 1.332e-003

Ca+2 1.279e-003 9.406e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.777e-005 3.498e-005 -4.423 -4.456 -0.033

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

CaCO3 2.921e-006 2.925e-006 -5.534 -5.534 0.001

CaOH+ 2.677e-009 2.474e-009 -8.572 -8.607 -0.034

CaHSO4+ 4.612e-012 4.263e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 6.065e-026

H2 3.032e-026 3.036e-026 -25.518 -25.518 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

KOH 1.684e-013 1.687e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

MgSO4 5.087e-006 5.094e-006 -5.294 -5.293 0.001

MgCO3 6.573e-007 6.581e-007 -6.182 -6.182 0.001

MgOH+ 1.164e-008 1.076e-008 -7.934 -7.968 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.723e-008 1.725e-008 -7.764 -7.763 0.001

NaSO4- 3.425e-009 3.166e-009 -8.465 -8.500 -0.034

NaCO3- 2.679e-010 2.476e-010 -9.572 -9.606 -0.034

NaOH 9.658e-013 9.671e-013 -12.015 -12.015 0.001

O(0) 4.039e-004

O2 2.019e-004 2.022e-004 -3.695 -3.694 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.253e-005 1.255e-005 -4.902 -4.901 0.001

MgSO4 5.087e-006 5.094e-006 -5.294 -5.293 0.001

NaSO4- 3.425e-009 3.166e-009 -8.465 -8.500 -0.034

KSO4- 1.469e-009 1.357e-009 -8.833 -8.867 -0.034

HSO4- 4.079e-010 3.770e-010 -9.389 -9.424 -0.034

CaHSO4+ 4.612e-012 4.263e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.38 CO2

Dolomite -0.90 -17.82 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.86 -3.69 -2.84 O2

Initial solution 8. 29/8/2012 13:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.095e-004 4.095e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.160

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.609e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.219e-003

Total CO2 (mol/kg) = 4.219e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.01

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551917e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0579 0.8112

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.828e-008 8.150e-008 -7.054 -7.089 -0.035

H+ 7.428e-008 6.918e-008 -7.129 -7.160 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.219e-003

HCO3- 3.587e-003 3.322e-003 -2.445 -2.479 -0.033

CO2 5.739e-004 5.746e-004 -3.241 -3.241 0.001

CaHCO3+ 3.779e-005 3.500e-005 -4.423 -4.456 -0.033

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

CaCO3 2.665e-006 2.669e-006 -5.574 -5.574 0.001

CO3-2 2.603e-006 1.916e-006 -5.585 -5.718 -0.133

MgCO3 5.997e-007 6.004e-007 -6.222 -6.222 0.001

NaHCO3 1.723e-008 1.725e-008 -7.764 -7.763 0.001

NaCO3- 2.444e-010 2.259e-010 -9.612 -9.646 -0.034

Ca 1.332e-003

Ca+2 1.279e-003 9.408e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.779e-005 3.500e-005 -4.423 -4.456 -0.033

CaSO4 1.254e-005 1.255e-005 -4.902 -4.901 0.001

CaCO3 2.665e-006 2.669e-006 -5.574 -5.574 0.001

CaOH+ 2.442e-009 2.257e-009 -8.612 -8.647 -0.034

CaHSO4+ 5.058e-012 4.675e-012 -11.296 -11.330 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 7.292e-026

H2 3.646e-026 3.651e-026 -25.438 -25.438 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.867 -0.034

KOH 1.536e-013 1.538e-013 -12.814 -12.813 0.001

Mg 5.184e-004

Mg+2 4.977e-004 3.675e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

MgSO4 5.088e-006 5.094e-006 -5.293 -5.293 0.001

MgCO3 5.997e-007 6.004e-007 -6.222 -6.222 0.001

MgOH+ 1.061e-008 9.811e-009 -7.974 -8.008 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.723e-008 1.725e-008 -7.764 -7.763 0.001

NaSO4- 3.425e-009 3.166e-009 -8.465 -8.500 -0.034

NaCO3- 2.444e-010 2.259e-010 -9.612 -9.646 -0.034

NaOH 8.809e-013 8.820e-013 -12.055 -12.055 0.001

O(0) 4.095e-004

O2 2.048e-004 2.050e-004 -3.689 -3.688 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.255e-005 -4.902 -4.901 0.001

MgSO4 5.088e-006 5.094e-006 -5.293 -5.293 0.001

NaSO4- 3.425e-009 3.166e-009 -8.465 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.867 -0.034

HSO4- 4.472e-010 4.133e-010 -9.349 -9.384 -0.034

CaHSO4+ 5.058e-012 4.675e-012 -11.296 -11.330 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.45 -8.74 -8.29 CaCO3

Calcite -0.30 -8.74 -8.44 CaCO3

CO2(g) -1.86 -3.24 -1.38 CO2

Dolomite -0.98 -17.90 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.32 -25.44 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.85 -3.69 -2.84 O2

Initial solution 9. 29/8/2012 13:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.208e-004 4.208e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.157e-003

Total CO2 (mol/kg) = 4.157e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551907e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0096 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.005e-007 9.281e-008 -6.998 -7.032 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.157e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.019e-004 5.025e-004 -3.299 -3.299 0.001

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CO3-2 2.989e-006 2.199e-006 -5.524 -5.658 -0.133

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.537e-026

H2 2.769e-026 2.772e-026 -25.558 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

MgOH+ 1.207e-008 1.115e-008 -7.918 -7.953 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.208e-004

O2 2.104e-004 2.107e-004 -3.677 -3.676 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.886e-010 3.592e-010 -9.410 -9.445 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.68 -2.83 O2

Initial solution 10. 29/8/2012 14:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.026e-004 4.026e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.157e-003

Total CO2 (mol/kg) = 4.157e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0048 0.8079

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.005e-007 9.281e-008 -6.998 -7.032 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.157e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.019e-004 5.025e-004 -3.299 -3.299 0.001

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CO3-2 2.989e-006 2.199e-006 -5.524 -5.658 -0.133

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.537e-026

H2 2.769e-026 2.772e-026 -25.558 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

MgOH+ 1.207e-008 1.115e-008 -7.918 -7.953 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.026e-004

O2 2.013e-004 2.016e-004 -3.696 -3.696 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.886e-010 3.592e-010 -9.410 -9.445 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 11. 29/8/2012 14:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.089e-004 4.089e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551908e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0164 0.8086

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.825e-008 9.069e-008 -7.008 -7.042 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.136e-004 5.143e-004 -3.289 -3.289 0.001

CaHCO3+ 3.789e-005 3.509e-005 -4.421 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 2.993e-006 2.997e-006 -5.524 -5.523 0.001

CO3-2 2.921e-006 2.149e-006 -5.534 -5.668 -0.133

MgCO3 6.715e-007 6.724e-007 -6.173 -6.172 0.001

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaCO3- 2.728e-010 2.521e-010 -9.564 -9.598 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.789e-005 3.509e-005 -4.421 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 2.993e-006 2.997e-006 -5.524 -5.523 0.001

CaOH+ 2.746e-009 2.538e-009 -8.561 -8.596 -0.034

CaHSO4+ 4.509e-012 4.167e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.798e-026

H2 2.899e-026 2.903e-026 -25.538 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.465e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.724e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.715e-007 6.724e-007 -6.173 -6.172 0.001

MgOH+ 1.179e-008 1.090e-008 -7.928 -7.963 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.728e-010 2.521e-010 -9.564 -9.598 -0.034

NaOH 9.883e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 4.089e-004

O2 2.044e-004 2.047e-004 -3.689 -3.689 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.465e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.977e-010 3.675e-010 -9.400 -9.435 -0.034

CaHSO4+ 4.509e-012 4.167e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.38 CO2

Dolomite -0.88 -17.80 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.69 -2.83 O2

Initial solution 12. 29/8/2012 14:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.189e-004 4.189e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.157e-003

Total CO2 (mol/kg) = 4.157e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551907e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0091 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.005e-007 9.281e-008 -6.998 -7.032 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.157e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.019e-004 5.025e-004 -3.299 -3.299 0.001

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CO3-2 2.989e-006 2.199e-006 -5.524 -5.658 -0.133

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.537e-026

H2 2.769e-026 2.772e-026 -25.558 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

MgOH+ 1.207e-008 1.115e-008 -7.918 -7.953 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.189e-004

O2 2.094e-004 2.097e-004 -3.679 -3.678 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.886e-010 3.592e-010 -9.410 -9.445 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.68 -2.83 O2

Initial solution 13. 29/8/2012 14:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.145e-004 4.145e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0279 0.8092

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.601e-008 8.863e-008 -7.018 -7.052 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.596e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.256e-004 5.263e-004 -3.279 -3.279 0.001

CaHCO3+ 3.790e-005 3.510e-005 -4.421 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 2.926e-006 2.929e-006 -5.534 -5.533 0.001

CO3-2 2.855e-006 2.101e-006 -5.544 -5.678 -0.133

MgCO3 6.563e-007 6.572e-007 -6.183 -6.182 0.001

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaCO3- 2.666e-010 2.464e-010 -9.574 -9.608 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.790e-005 3.510e-005 -4.421 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 2.926e-006 2.929e-006 -5.534 -5.533 0.001

CaOH+ 2.684e-009 2.480e-009 -8.571 -8.606 -0.034

CaHSO4+ 4.614e-012 4.264e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.071e-026

H2 3.036e-026 3.040e-026 -25.518 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.465e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.563e-007 6.572e-007 -6.183 -6.182 0.001

MgOH+ 1.153e-008 1.065e-008 -7.938 -7.973 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.666e-010 2.464e-010 -9.574 -9.608 -0.034

NaOH 9.658e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 4.145e-004

O2 2.073e-004 2.075e-004 -3.684 -3.683 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.465e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 4.070e-010 3.761e-010 -9.390 -9.425 -0.034

CaHSO4+ 4.614e-012 4.264e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.38 CO2

Dolomite -0.90 -17.82 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.68 -2.83 O2

Initial solution 14. 29/8/2012 15:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.014e-004 4.014e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.192e-003

Total CO2 (mol/kg) = 4.192e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551913e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0244 0.8090

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.602e-008 8.863e-008 -7.018 -7.052 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.192e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.270e-004 5.277e-004 -3.278 -3.278 0.001

CaHCO3+ 3.809e-005 3.528e-005 -4.419 -4.452 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.941e-006 2.944e-006 -5.532 -5.531 0.001

CO3-2 2.863e-006 2.106e-006 -5.543 -5.676 -0.133

MgCO3 6.579e-007 6.587e-007 -6.182 -6.181 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.673e-010 2.470e-010 -9.573 -9.607 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.453e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.809e-005 3.528e-005 -4.419 -4.452 -0.033

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

CaCO3 2.941e-006 2.944e-006 -5.532 -5.531 0.001

CaOH+ 2.690e-009 2.486e-009 -8.570 -8.604 -0.034

CaHSO4+ 4.623e-012 4.272e-012 -11.335 -11.369 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.071e-026

H2 3.036e-026 3.040e-026 -25.518 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.465e-009 1.354e-009 -8.834 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.066e-006 5.073e-006 -5.295 -5.295 0.001

MgCO3 6.579e-007 6.587e-007 -6.182 -6.181 0.001

MgOH+ 1.152e-008 1.065e-008 -7.938 -7.973 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.420e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.673e-010 2.470e-010 -9.573 -9.607 -0.034

NaOH 9.657e-013 9.669e-013 -12.015 -12.015 0.001

O(0) 4.014e-004

O2 2.007e-004 2.009e-004 -3.697 -3.697 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

MgSO4 5.066e-006 5.073e-006 -5.295 -5.295 0.001

NaSO4- 3.420e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.465e-009 1.354e-009 -8.834 -8.869 -0.034

HSO4- 4.068e-010 3.759e-010 -9.391 -9.425 -0.034

CaHSO4+ 4.623e-012 4.272e-012 -11.335 -11.369 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.38 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 15. 29/8/2012 15:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.982e-004 3.982e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551910e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0223 0.8086

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.159e-004 5.165e-004 -3.287 -3.287 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CO3-2 2.923e-006 2.150e-006 -5.534 -5.668 -0.133

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CaOH+ 2.753e-009 2.544e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 3.982e-004

O2 1.991e-004 1.994e-004 -3.701 -3.700 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.968e-010 3.667e-010 -9.401 -9.436 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.70 -2.83 O2

Initial solution 16. 29/8/2012 15:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.033e-004 4.033e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.160

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.634e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.245e-003

Total CO2 (mol/kg) = 4.245e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551924e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0737 0.8116

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.686e-008 8.017e-008 -7.061 -7.096 -0.035

H+ 7.429e-008 6.918e-008 -7.129 -7.160 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.245e-003

HCO3- 3.607e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.790e-004 5.798e-004 -3.237 -3.237 0.001

CaHCO3+ 3.804e-005 3.523e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.397e-005 -4.821 -4.855 -0.034

CaCO3 2.673e-006 2.677e-006 -5.573 -5.572 0.001

CO3-2 2.606e-006 1.917e-006 -5.584 -5.717 -0.133

MgCO3 5.979e-007 5.987e-007 -6.223 -6.223 0.001

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaCO3- 2.420e-010 2.236e-010 -9.616 -9.650 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.456e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.804e-005 3.523e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.673e-006 2.677e-006 -5.573 -5.572 0.001

CaOH+ 2.454e-009 2.268e-009 -8.610 -8.644 -0.034

CaHSO4+ 5.061e-012 4.677e-012 -11.296 -11.330 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 7.307e-026

H2 3.653e-026 3.658e-026 -25.437 -25.437 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.536e-013 1.538e-013 -12.814 -12.813 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.397e-005 -4.821 -4.855 -0.034

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 5.979e-007 5.987e-007 -6.223 -6.223 0.001

MgOH+ 1.041e-008 9.621e-009 -7.983 -8.017 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

NaCO3- 2.420e-010 2.236e-010 -9.616 -9.650 -0.034

NaOH 8.807e-013 8.819e-013 -12.055 -12.055 0.001

O(0) 4.033e-004

O2 2.016e-004 2.019e-004 -3.695 -3.695 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.452e-010 4.114e-010 -9.351 -9.386 -0.034

CaHSO4+ 5.061e-012 4.677e-012 -11.296 -11.330 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.45 -8.74 -8.29 CaCO3

Calcite -0.30 -8.74 -8.44 CaCO3

CO2(g) -1.86 -3.24 -1.37 CO2

Dolomite -0.98 -17.89 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.32 -25.44 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.69 -2.83 O2

Initial solution 17. 29/8/2012 15:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.939e-004 3.939e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.193e-003

Total CO2 (mol/kg) = 4.193e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551912e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0311 0.8091

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.193e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.279e-004 5.286e-004 -3.277 -3.277 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CO3-2 2.856e-006 2.101e-006 -5.544 -5.678 -0.133

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CaOH+ 2.691e-009 2.486e-009 -8.570 -8.604 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

MgOH+ 1.141e-008 1.055e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

NaOH 9.657e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 3.939e-004

O2 1.969e-004 1.972e-004 -3.706 -3.705 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.061e-010 3.752e-010 -9.391 -9.426 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.71 -2.83 O2

Initial solution 18. 29/8/2012 16:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.882e-004 3.882e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.193e-003

Total CO2 (mol/kg) = 4.193e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551912e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0295 0.8091

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.193e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.279e-004 5.286e-004 -3.277 -3.277 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CO3-2 2.856e-006 2.101e-006 -5.544 -5.678 -0.133

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CaOH+ 2.691e-009 2.486e-009 -8.570 -8.604 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

MgOH+ 1.141e-008 1.055e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

NaOH 9.657e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 3.882e-004

O2 1.941e-004 1.944e-004 -3.712 -3.711 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.061e-010 3.752e-010 -9.391 -9.426 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 19. 29/8/2012 16:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.876e-004 3.876e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.160

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.634e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.245e-003

Total CO2 (mol/kg) = 4.245e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551922e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0694 0.8114

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.686e-008 8.017e-008 -7.061 -7.096 -0.035

H+ 7.429e-008 6.918e-008 -7.129 -7.160 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.245e-003

HCO3- 3.607e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.790e-004 5.798e-004 -3.237 -3.237 0.001

CaHCO3+ 3.804e-005 3.523e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.397e-005 -4.821 -4.855 -0.034

CaCO3 2.673e-006 2.677e-006 -5.573 -5.572 0.001

CO3-2 2.606e-006 1.917e-006 -5.584 -5.717 -0.133

MgCO3 5.979e-007 5.987e-007 -6.223 -6.223 0.001

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaCO3- 2.420e-010 2.236e-010 -9.616 -9.650 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.456e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.804e-005 3.523e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.673e-006 2.677e-006 -5.573 -5.572 0.001

CaOH+ 2.454e-009 2.268e-009 -8.610 -8.644 -0.034

CaHSO4+ 5.061e-012 4.677e-012 -11.296 -11.330 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 7.307e-026

H2 3.653e-026 3.658e-026 -25.437 -25.437 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.536e-013 1.538e-013 -12.814 -12.813 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.397e-005 -4.821 -4.855 -0.034

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 5.979e-007 5.987e-007 -6.223 -6.223 0.001

MgOH+ 1.041e-008 9.621e-009 -7.983 -8.017 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

NaCO3- 2.420e-010 2.236e-010 -9.616 -9.650 -0.034

NaOH 8.807e-013 8.819e-013 -12.055 -12.055 0.001

O(0) 3.876e-004

O2 1.938e-004 1.941e-004 -3.713 -3.712 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.452e-010 4.114e-010 -9.351 -9.386 -0.034

CaHSO4+ 5.061e-012 4.677e-012 -11.296 -11.330 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.45 -8.74 -8.29 CaCO3

Calcite -0.30 -8.74 -8.44 CaCO3

CO2(g) -1.86 -3.24 -1.37 CO2

Dolomite -0.98 -17.89 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.32 -25.44 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 20. 29/8/2012 16:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.682e-003 3.682e-003

Ca 1.343e-003 1.343e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.751e-004 3.751e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.645e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.205e-003

Total CO2 (mol/kg) = 4.205e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.335e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.11

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551914e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0258 0.8088

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.776e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.205e-003

HCO3- 3.616e-003 3.348e-003 -2.442 -2.475 -0.033

CO2 5.293e-004 5.300e-004 -3.276 -3.276 0.001

CaHCO3+ 3.822e-005 3.539e-005 -4.418 -4.451 -0.033

MgHCO3+ 1.514e-005 1.399e-005 -4.820 -4.854 -0.034

CaCO3 2.945e-006 2.949e-006 -5.531 -5.530 0.001

CO3-2 2.865e-006 2.107e-006 -5.543 -5.676 -0.133

MgCO3 6.569e-007 6.577e-007 -6.183 -6.182 0.001

NaHCO3 1.737e-008 1.739e-008 -7.760 -7.760 0.001

NaCO3- 2.660e-010 2.458e-010 -9.575 -9.609 -0.034

Ca 1.343e-003

Ca+2 1.289e-003 9.477e-004 -2.890 -3.023 -0.134

CaHCO3+ 3.822e-005 3.539e-005 -4.418 -4.451 -0.033

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

CaCO3 2.945e-006 2.949e-006 -5.531 -5.530 0.001

CaOH+ 2.697e-009 2.493e-009 -8.569 -8.603 -0.034

CaHSO4+ 4.625e-012 4.273e-012 -11.335 -11.369 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.671e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.514e-005 1.399e-005 -4.820 -4.854 -0.034

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

MgCO3 6.569e-007 6.577e-007 -6.183 -6.182 0.001

MgOH+ 1.141e-008 1.054e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.986e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.737e-008 1.739e-008 -7.760 -7.760 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.660e-010 2.458e-010 -9.575 -9.609 -0.034

NaOH 9.656e-013 9.669e-013 -12.015 -12.015 0.001

O(0) 3.751e-004

O2 1.876e-004 1.878e-004 -3.727 -3.726 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.164e-005 -4.010 -4.145 -0.135

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.059e-010 3.751e-010 -9.392 -9.426 -0.034

CaHSO4+ 4.625e-012 4.273e-012 -11.335 -11.369 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.73 -2.83 O2

Initial solution 21. 29/8/2012 16:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.682e-003 3.682e-003

Ca 1.343e-003 1.343e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.776e-004 3.776e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.190

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.645e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.217e-003

Total CO2 (mol/kg) = 4.217e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.335e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.11

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551917e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0365 0.8095

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.307e-008 8.591e-008 -7.031 -7.066 -0.035

H+ 6.934e-008 6.457e-008 -7.159 -7.190 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.217e-003

HCO3- 3.616e-003 3.349e-003 -2.442 -2.475 -0.033

CO2 5.417e-004 5.424e-004 -3.266 -3.266 0.001

CaHCO3+ 3.822e-005 3.540e-005 -4.418 -4.451 -0.033

MgHCO3+ 1.515e-005 1.400e-005 -4.820 -4.854 -0.034

CaCO3 2.878e-006 2.882e-006 -5.541 -5.540 0.001

CO3-2 2.800e-006 2.059e-006 -5.553 -5.686 -0.133

MgCO3 6.420e-007 6.428e-007 -6.192 -6.192 0.001

NaHCO3 1.737e-008 1.739e-008 -7.760 -7.760 0.001

NaCO3- 2.599e-010 2.402e-010 -9.585 -9.619 -0.034

Ca 1.343e-003

Ca+2 1.290e-003 9.478e-004 -2.890 -3.023 -0.134

CaHCO3+ 3.822e-005 3.540e-005 -4.418 -4.451 -0.033

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

CaCO3 2.878e-006 2.882e-006 -5.541 -5.540 0.001

CaOH+ 2.636e-009 2.436e-009 -8.579 -8.613 -0.034

CaHSO4+ 4.733e-012 4.373e-012 -11.325 -11.359 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.364e-026

H2 3.182e-026 3.186e-026 -25.497 -25.497 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.646e-013 1.648e-013 -12.784 -12.783 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.671e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.515e-005 1.400e-005 -4.820 -4.854 -0.034

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

MgCO3 6.420e-007 6.428e-007 -6.192 -6.192 0.001

MgOH+ 1.115e-008 1.030e-008 -7.953 -7.987 -0.034

Na 1.001e-005

Na+ 9.986e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.737e-008 1.739e-008 -7.760 -7.760 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.599e-010 2.402e-010 -9.585 -9.619 -0.034

NaOH 9.436e-013 9.449e-013 -12.025 -12.025 0.001

O(0) 3.776e-004

O2 1.888e-004 1.891e-004 -3.724 -3.723 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.164e-005 -4.010 -4.145 -0.135

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.153e-010 3.838e-010 -9.382 -9.416 -0.034

CaHSO4+ 4.733e-012 4.373e-012 -11.325 -11.359 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.42 -8.71 -8.29 CaCO3

Calcite -0.27 -8.71 -8.44 CaCO3

CO2(g) -1.89 -3.27 -1.37 CO2

Dolomite -0.92 -17.83 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.38 -25.50 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 22. 29/8/2012 17:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.682e-003 3.682e-003

Ca 1.343e-003 1.343e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.695e-004 3.695e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.645e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.193e-003

Total CO2 (mol/kg) = 4.193e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.335e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.11

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0142 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.746e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.193e-003

HCO3- 3.615e-003 3.348e-003 -2.442 -2.475 -0.033

CO2 5.173e-004 5.179e-004 -3.286 -3.286 0.001

CaHCO3+ 3.821e-005 3.539e-005 -4.418 -4.451 -0.033

MgHCO3+ 1.514e-005 1.399e-005 -4.820 -4.854 -0.034

CaCO3 3.013e-006 3.017e-006 -5.521 -5.520 0.001

CO3-2 2.931e-006 2.156e-006 -5.533 -5.666 -0.133

MgCO3 6.721e-007 6.730e-007 -6.173 -6.172 0.001

NaHCO3 1.736e-008 1.739e-008 -7.760 -7.760 0.001

NaCO3- 2.721e-010 2.515e-010 -9.565 -9.600 -0.034

Ca 1.343e-003

Ca+2 1.289e-003 9.477e-004 -2.890 -3.023 -0.134

CaHCO3+ 3.821e-005 3.539e-005 -4.418 -4.451 -0.033

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

CaCO3 3.013e-006 3.017e-006 -5.521 -5.520 0.001

CaOH+ 2.760e-009 2.550e-009 -8.559 -8.593 -0.034

CaHSO4+ 4.519e-012 4.176e-012 -11.345 -11.379 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.671e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.514e-005 1.399e-005 -4.820 -4.854 -0.034

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

MgCO3 6.721e-007 6.730e-007 -6.173 -6.172 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.986e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.736e-008 1.739e-008 -7.760 -7.760 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.721e-010 2.515e-010 -9.565 -9.600 -0.034

NaOH 9.881e-013 9.894e-013 -12.005 -12.005 0.001

O(0) 3.695e-004

O2 1.847e-004 1.850e-004 -3.733 -3.733 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.164e-005 -4.010 -4.145 -0.135

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.966e-010 3.665e-010 -9.402 -9.436 -0.034

CaHSO4+ 4.519e-012 4.176e-012 -11.345 -11.379 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.90 -3.73 -2.83 O2

Initial solution 23. 29/8/2012 17:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.807e-004 3.807e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551906e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0074 0.8078

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.807e-004

O2 1.904e-004 1.906e-004 -3.720 -3.720 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 24. 29/8/2012 17:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.682e-003 3.682e-003

Ca 1.343e-003 1.343e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.007e-004 4.007e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.645e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.205e-003

Total CO2 (mol/kg) = 4.205e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.335e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.11

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551916e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0330 0.8093

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.776e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.205e-003

HCO3- 3.616e-003 3.348e-003 -2.442 -2.475 -0.033

CO2 5.293e-004 5.300e-004 -3.276 -3.276 0.001

CaHCO3+ 3.822e-005 3.539e-005 -4.418 -4.451 -0.033

MgHCO3+ 1.514e-005 1.399e-005 -4.820 -4.854 -0.034

CaCO3 2.945e-006 2.949e-006 -5.531 -5.530 0.001

CO3-2 2.865e-006 2.107e-006 -5.543 -5.676 -0.133

MgCO3 6.569e-007 6.577e-007 -6.183 -6.182 0.001

NaHCO3 1.737e-008 1.739e-008 -7.760 -7.760 0.001

NaCO3- 2.660e-010 2.458e-010 -9.575 -9.609 -0.034

Ca 1.343e-003

Ca+2 1.289e-003 9.477e-004 -2.890 -3.023 -0.134

CaHCO3+ 3.822e-005 3.539e-005 -4.418 -4.451 -0.033

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

CaCO3 2.945e-006 2.949e-006 -5.531 -5.530 0.001

CaOH+ 2.697e-009 2.493e-009 -8.569 -8.603 -0.034

CaHSO4+ 4.625e-012 4.273e-012 -11.335 -11.369 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.671e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.514e-005 1.399e-005 -4.820 -4.854 -0.034

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

MgCO3 6.569e-007 6.577e-007 -6.183 -6.182 0.001

MgOH+ 1.141e-008 1.054e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.986e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.737e-008 1.739e-008 -7.760 -7.760 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.660e-010 2.458e-010 -9.575 -9.609 -0.034

NaOH 9.656e-013 9.669e-013 -12.015 -12.015 0.001

O(0) 4.007e-004

O2 2.004e-004 2.006e-004 -3.698 -3.698 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.164e-005 -4.010 -4.145 -0.135

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.059e-010 3.751e-010 -9.392 -9.426 -0.034

CaHSO4+ 4.625e-012 4.273e-012 -11.335 -11.369 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 25. 29/8/2012 17:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.826e-004 3.826e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551906e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0080 0.8078

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.826e-004

O2 1.913e-004 1.916e-004 -3.718 -3.718 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.72 -2.83 O2

Initial solution 26. 29/8/2012 18:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.901e-004 3.901e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551910e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0201 0.8085

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.159e-004 5.165e-004 -3.287 -3.287 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CO3-2 2.923e-006 2.150e-006 -5.534 -5.668 -0.133

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CaOH+ 2.753e-009 2.544e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 3.901e-004

O2 1.951e-004 1.953e-004 -3.710 -3.709 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.968e-010 3.667e-010 -9.401 -9.436 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 27. 29/8/2012 18:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.814e-004 3.814e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.193e-003

Total CO2 (mol/kg) = 4.193e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0276 0.8089

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.193e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.279e-004 5.286e-004 -3.277 -3.277 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CO3-2 2.856e-006 2.101e-006 -5.544 -5.678 -0.133

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CaOH+ 2.691e-009 2.486e-009 -8.570 -8.604 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

MgOH+ 1.141e-008 1.055e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

NaOH 9.657e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 3.814e-004

O2 1.907e-004 1.909e-004 -3.720 -3.719 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.061e-010 3.752e-010 -9.391 -9.426 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 28. 29/8/2012 18:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.751e-004 3.751e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.190

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.206e-003

Total CO2 (mol/kg) = 4.206e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551913e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0358 0.8094

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.307e-008 8.591e-008 -7.031 -7.066 -0.035

H+ 6.933e-008 6.457e-008 -7.159 -7.190 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.206e-003

HCO3- 3.606e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.403e-004 5.410e-004 -3.267 -3.267 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CO3-2 2.792e-006 2.054e-006 -5.554 -5.687 -0.133

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CaOH+ 2.630e-009 2.430e-009 -8.580 -8.614 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.364e-026

H2 3.182e-026 3.186e-026 -25.497 -25.497 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.646e-013 1.648e-013 -12.784 -12.783 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

MgOH+ 1.115e-008 1.031e-008 -7.953 -7.987 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

NaOH 9.437e-013 9.449e-013 -12.025 -12.025 0.001

O(0) 3.751e-004

O2 1.876e-004 1.878e-004 -3.727 -3.726 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.155e-010 3.840e-010 -9.381 -9.416 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.42 -8.71 -8.29 CaCO3

Calcite -0.27 -8.71 -8.44 CaCO3

CO2(g) -1.89 -3.27 -1.37 CO2

Dolomite -0.92 -17.83 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.38 -25.50 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.73 -2.83 O2

Initial solution 29. 29/8/2012 18:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.682e-003 3.682e-003

Ca 1.343e-003 1.343e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.870e-004 3.870e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.645e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.205e-003

Total CO2 (mol/kg) = 4.205e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.335e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.11

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551915e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0292 0.8090

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.776e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.205e-003

HCO3- 3.616e-003 3.348e-003 -2.442 -2.475 -0.033

CO2 5.293e-004 5.300e-004 -3.276 -3.276 0.001

CaHCO3+ 3.822e-005 3.539e-005 -4.418 -4.451 -0.033

MgHCO3+ 1.514e-005 1.399e-005 -4.820 -4.854 -0.034

CaCO3 2.945e-006 2.949e-006 -5.531 -5.530 0.001

CO3-2 2.865e-006 2.107e-006 -5.543 -5.676 -0.133

MgCO3 6.569e-007 6.577e-007 -6.183 -6.182 0.001

NaHCO3 1.737e-008 1.739e-008 -7.760 -7.760 0.001

NaCO3- 2.660e-010 2.458e-010 -9.575 -9.609 -0.034

Ca 1.343e-003

Ca+2 1.289e-003 9.477e-004 -2.890 -3.023 -0.134

CaHCO3+ 3.822e-005 3.539e-005 -4.418 -4.451 -0.033

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

CaCO3 2.945e-006 2.949e-006 -5.531 -5.530 0.001

CaOH+ 2.697e-009 2.493e-009 -8.569 -8.603 -0.034

CaHSO4+ 4.625e-012 4.273e-012 -11.335 -11.369 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.671e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.514e-005 1.399e-005 -4.820 -4.854 -0.034

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

MgCO3 6.569e-007 6.577e-007 -6.183 -6.182 0.001

MgOH+ 1.141e-008 1.054e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.986e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.737e-008 1.739e-008 -7.760 -7.760 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.660e-010 2.458e-010 -9.575 -9.609 -0.034

NaOH 9.656e-013 9.669e-013 -12.015 -12.015 0.001

O(0) 3.870e-004

O2 1.935e-004 1.937e-004 -3.713 -3.713 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.164e-005 -4.010 -4.145 -0.135

CaSO4 1.259e-005 1.261e-005 -4.900 -4.899 0.001

MgSO4 5.050e-006 5.057e-006 -5.297 -5.296 0.001

NaSO4- 3.417e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.059e-010 3.751e-010 -9.392 -9.426 -0.034

CaHSO4+ 4.625e-012 4.273e-012 -11.335 -11.369 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 30. 29/8/2012 19:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.964e-004 3.964e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551908e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0118 0.8080

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.964e-004

O2 1.982e-004 1.984e-004 -3.703 -3.702 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.70 -2.83 O2

Initial solution 31. 29/8/2012 19:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.826e-004 3.826e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.193e-003

Total CO2 (mol/kg) = 4.193e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0280 0.8090

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.193e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.279e-004 5.286e-004 -3.277 -3.277 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CO3-2 2.856e-006 2.101e-006 -5.544 -5.678 -0.133

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CaOH+ 2.691e-009 2.486e-009 -8.570 -8.604 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

MgOH+ 1.141e-008 1.055e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

NaOH 9.657e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 3.826e-004

O2 1.913e-004 1.916e-004 -3.718 -3.718 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.061e-010 3.752e-010 -9.391 -9.426 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.72 -2.83 O2

Initial solution 32. 29/8/2012 19:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.895e-004 3.895e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.110

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.635e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.317e-003

Total CO2 (mol/kg) = 4.317e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551937e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.1199 0.8143

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

H+ 8.335e-008 7.762e-008 -7.079 -7.110 -0.031

OH- 7.741e-008 7.145e-008 -7.111 -7.146 -0.035

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.317e-003

HCO3- 3.608e-003 3.342e-003 -2.443 -2.476 -0.033

CO2 6.499e-004 6.508e-004 -3.187 -3.187 0.001

CaHCO3+ 3.806e-005 3.525e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.512e-005 1.397e-005 -4.820 -4.855 -0.034

CaCO3 2.384e-006 2.387e-006 -5.623 -5.622 0.001

CO3-2 2.323e-006 1.709e-006 -5.634 -5.767 -0.133

MgCO3 5.331e-007 5.338e-007 -6.273 -6.273 0.001

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaCO3- 2.158e-010 1.994e-010 -9.666 -9.700 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.458e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.806e-005 3.525e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

CaCO3 2.384e-006 2.387e-006 -5.623 -5.622 0.001

CaOH+ 2.188e-009 2.022e-009 -8.660 -8.694 -0.034

CaHSO4+ 5.680e-012 5.249e-012 -11.246 -11.280 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 9.199e-026

H2 4.599e-026 4.605e-026 -25.337 -25.337 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.369e-013 1.371e-013 -12.864 -12.863 0.001

Mg 5.184e-004

Mg+2 4.977e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.512e-005 1.397e-005 -4.820 -4.855 -0.034

MgSO4 5.055e-006 5.062e-006 -5.296 -5.296 0.001

MgCO3 5.331e-007 5.338e-007 -6.273 -6.273 0.001

MgOH+ 9.280e-009 8.575e-009 -8.032 -8.067 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

NaCO3- 2.158e-010 1.994e-010 -9.666 -9.700 -0.034

NaOH 7.849e-013 7.860e-013 -12.105 -12.105 0.001

O(0) 3.895e-004

O2 1.947e-004 1.950e-004 -3.711 -3.710 0.001

S(6) 1.154e-004

SO4-2 9.774e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

MgSO4 5.055e-006 5.062e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.995e-010 4.616e-010 -9.301 -9.336 -0.034

CaHSO4+ 5.680e-012 5.249e-012 -11.246 -11.280 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.50 -8.79 -8.29 CaCO3

Calcite -0.35 -8.79 -8.44 CaCO3

CO2(g) -1.81 -3.19 -1.37 CO2

Dolomite -1.08 -17.99 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.22 -25.34 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 33. 29/8/2012 19:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.189e-004 4.189e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.190

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.206e-003

Total CO2 (mol/kg) = 4.206e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551917e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0478 0.8101

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.307e-008 8.591e-008 -7.031 -7.066 -0.035

H+ 6.933e-008 6.457e-008 -7.159 -7.190 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.206e-003

HCO3- 3.606e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.403e-004 5.410e-004 -3.267 -3.267 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CO3-2 2.792e-006 2.054e-006 -5.554 -5.687 -0.133

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CaOH+ 2.630e-009 2.430e-009 -8.580 -8.614 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.364e-026

H2 3.182e-026 3.186e-026 -25.497 -25.497 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.646e-013 1.648e-013 -12.784 -12.783 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

MgOH+ 1.115e-008 1.031e-008 -7.953 -7.987 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

NaOH 9.437e-013 9.449e-013 -12.025 -12.025 0.001

O(0) 4.189e-004

O2 2.094e-004 2.097e-004 -3.679 -3.678 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.155e-010 3.840e-010 -9.381 -9.416 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.42 -8.71 -8.29 CaCO3

Calcite -0.27 -8.71 -8.44 CaCO3

CO2(g) -1.89 -3.27 -1.37 CO2

Dolomite -0.92 -17.83 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.38 -25.50 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.68 -2.83 O2

Initial solution 34. 29/8/2012 20:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.801e-004 3.801e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551909e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0172 0.8083

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.159e-004 5.165e-004 -3.287 -3.287 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CO3-2 2.923e-006 2.150e-006 -5.534 -5.668 -0.133

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CaOH+ 2.753e-009 2.544e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 3.801e-004

O2 1.901e-004 1.903e-004 -3.721 -3.721 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.968e-010 3.667e-010 -9.401 -9.436 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 35. 29/8/2012 20:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.114e-004 4.114e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.193e-003

Total CO2 (mol/kg) = 4.193e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551914e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0358 0.8094

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.193e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.279e-004 5.286e-004 -3.277 -3.277 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CO3-2 2.856e-006 2.101e-006 -5.544 -5.678 -0.133

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CaOH+ 2.691e-009 2.486e-009 -8.570 -8.604 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

MgOH+ 1.141e-008 1.055e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

NaOH 9.657e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 4.114e-004

O2 2.057e-004 2.060e-004 -3.687 -3.686 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.061e-010 3.752e-010 -9.391 -9.426 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.69 -2.83 O2

Initial solution 36. 29/8/2012 20:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.851e-004 3.851e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.190

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.206e-003

Total CO2 (mol/kg) = 4.206e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551914e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0387 0.8096

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.307e-008 8.591e-008 -7.031 -7.066 -0.035

H+ 6.933e-008 6.457e-008 -7.159 -7.190 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.206e-003

HCO3- 3.606e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.403e-004 5.410e-004 -3.267 -3.267 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CO3-2 2.792e-006 2.054e-006 -5.554 -5.687 -0.133

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CaOH+ 2.630e-009 2.430e-009 -8.580 -8.614 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.364e-026

H2 3.182e-026 3.186e-026 -25.497 -25.497 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.646e-013 1.648e-013 -12.784 -12.783 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

MgOH+ 1.115e-008 1.031e-008 -7.953 -7.987 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

NaOH 9.437e-013 9.449e-013 -12.025 -12.025 0.001

O(0) 3.851e-004

O2 1.926e-004 1.928e-004 -3.715 -3.715 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.155e-010 3.840e-010 -9.381 -9.416 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.42 -8.71 -8.29 CaCO3

Calcite -0.27 -8.71 -8.44 CaCO3

CO2(g) -1.89 -3.27 -1.37 CO2

Dolomite -0.92 -17.83 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.38 -25.50 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 37. 29/8/2012 20:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.907e-004 3.907e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.190

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.206e-003

Total CO2 (mol/kg) = 4.206e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551915e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0402 0.8097

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.307e-008 8.591e-008 -7.031 -7.066 -0.035

H+ 6.933e-008 6.457e-008 -7.159 -7.190 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.206e-003

HCO3- 3.606e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.403e-004 5.410e-004 -3.267 -3.267 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CO3-2 2.792e-006 2.054e-006 -5.554 -5.687 -0.133

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CaOH+ 2.630e-009 2.430e-009 -8.580 -8.614 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.364e-026

H2 3.182e-026 3.186e-026 -25.497 -25.497 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.646e-013 1.648e-013 -12.784 -12.783 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

MgOH+ 1.115e-008 1.031e-008 -7.953 -7.987 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

NaOH 9.437e-013 9.449e-013 -12.025 -12.025 0.001

O(0) 3.907e-004

O2 1.954e-004 1.956e-004 -3.709 -3.709 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.155e-010 3.840e-010 -9.381 -9.416 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.42 -8.71 -8.29 CaCO3

Calcite -0.27 -8.71 -8.44 CaCO3

CO2(g) -1.89 -3.27 -1.37 CO2

Dolomite -0.92 -17.83 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.38 -25.50 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.71 -2.83 O2

Initial solution 38. 29/8/2012 21:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.001e-004 4.001e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.190

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.206e-003

Total CO2 (mol/kg) = 4.206e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551916e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0428 0.8098

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.307e-008 8.591e-008 -7.031 -7.066 -0.035

H+ 6.933e-008 6.457e-008 -7.159 -7.190 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.206e-003

HCO3- 3.606e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.403e-004 5.410e-004 -3.267 -3.267 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CO3-2 2.792e-006 2.054e-006 -5.554 -5.687 -0.133

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CaOH+ 2.630e-009 2.430e-009 -8.580 -8.614 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.364e-026

H2 3.182e-026 3.186e-026 -25.497 -25.497 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.646e-013 1.648e-013 -12.784 -12.783 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

MgOH+ 1.115e-008 1.031e-008 -7.953 -7.987 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

NaOH 9.437e-013 9.449e-013 -12.025 -12.025 0.001

O(0) 4.001e-004

O2 2.001e-004 2.003e-004 -3.699 -3.698 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.155e-010 3.840e-010 -9.381 -9.416 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.42 -8.71 -8.29 CaCO3

Calcite -0.27 -8.71 -8.44 CaCO3

CO2(g) -1.89 -3.27 -1.37 CO2

Dolomite -0.92 -17.83 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.38 -25.50 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 39. 29/8/2012 21:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.170e-004 4.170e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.270

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.632e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.113e-003

Total CO2 (mol/kg) = 4.113e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551899e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9673 0.8055

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.119e-007 1.033e-007 -6.951 -6.986 -0.035

H+ 5.767e-008 5.370e-008 -7.239 -7.270 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.113e-003

HCO3- 3.604e-003 3.337e-003 -2.443 -2.477 -0.033

CO2 4.491e-004 4.497e-004 -3.348 -3.347 0.001

CaHCO3+ 3.799e-005 3.518e-005 -4.420 -4.454 -0.033

MgHCO3+ 1.510e-005 1.395e-005 -4.821 -4.855 -0.034

CaCO3 3.439e-006 3.444e-006 -5.464 -5.463 0.001

CO3-2 3.354e-006 2.467e-006 -5.474 -5.608 -0.133

MgCO3 7.694e-007 7.704e-007 -6.114 -6.113 0.001

NaHCO3 1.731e-008 1.733e-008 -7.762 -7.761 0.001

NaCO3- 3.115e-010 2.878e-010 -9.507 -9.541 -0.034

Ca 1.339e-003

Ca+2 1.285e-003 9.451e-004 -2.891 -3.025 -0.134

CaHCO3+ 3.799e-005 3.518e-005 -4.420 -4.454 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.439e-006 3.444e-006 -5.464 -5.463 0.001

CaOH+ 3.160e-009 2.920e-009 -8.500 -8.535 -0.034

CaHSO4+ 3.927e-012 3.629e-012 -11.406 -11.440 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 4.403e-026

H2 2.201e-026 2.204e-026 -25.657 -25.657 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.979e-013 1.981e-013 -12.704 -12.703 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.395e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.060e-006 -5.296 -5.296 0.001

MgCO3 7.694e-007 7.704e-007 -6.114 -6.113 0.001

MgOH+ 1.341e-008 1.239e-008 -7.873 -7.907 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.731e-008 1.733e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 3.115e-010 2.878e-010 -9.507 -9.541 -0.034

NaOH 1.135e-012 1.136e-012 -11.945 -11.945 0.001

O(0) 4.170e-004

O2 2.085e-004 2.088e-004 -3.681 -3.680 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.060e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.456e-010 3.194e-010 -9.461 -9.496 -0.034

CaHSO4+ 3.927e-012 3.629e-012 -11.406 -11.440 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.34 -8.63 -8.29 CaCO3

Calcite -0.19 -8.63 -8.44 CaCO3

CO2(g) -1.97 -3.35 -1.37 CO2

Dolomite -0.76 -17.68 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.54 -25.66 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.68 -2.83 O2

Initial solution 40. 29/8/2012 21:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.789e-004 3.789e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.190

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.206e-003

Total CO2 (mol/kg) = 4.206e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551913e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0369 0.8095

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.307e-008 8.591e-008 -7.031 -7.066 -0.035

H+ 6.933e-008 6.457e-008 -7.159 -7.190 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.206e-003

HCO3- 3.606e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.403e-004 5.410e-004 -3.267 -3.267 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CO3-2 2.792e-006 2.054e-006 -5.554 -5.687 -0.133

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.864e-006 2.867e-006 -5.543 -5.543 0.001

CaOH+ 2.630e-009 2.430e-009 -8.580 -8.614 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.364e-026

H2 3.182e-026 3.186e-026 -25.497 -25.497 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.646e-013 1.648e-013 -12.784 -12.783 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.405e-007 6.413e-007 -6.193 -6.193 0.001

MgOH+ 1.115e-008 1.031e-008 -7.953 -7.987 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.592e-010 2.396e-010 -9.586 -9.621 -0.034

NaOH 9.437e-013 9.449e-013 -12.025 -12.025 0.001

O(0) 3.789e-004

O2 1.894e-004 1.897e-004 -3.723 -3.722 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.155e-010 3.840e-010 -9.381 -9.416 -0.034

CaHSO4+ 4.723e-012 4.365e-012 -11.326 -11.360 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.42 -8.71 -8.29 CaCO3

Calcite -0.27 -8.71 -8.44 CaCO3

CO2(g) -1.89 -3.27 -1.37 CO2

Dolomite -0.92 -17.83 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.38 -25.50 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 41. 29/8/2012 21:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.757e-004 3.757e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.160

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.634e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.245e-003

Total CO2 (mol/kg) = 4.245e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551921e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0660 0.8112

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.686e-008 8.017e-008 -7.061 -7.096 -0.035

H+ 7.429e-008 6.918e-008 -7.129 -7.160 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.245e-003

HCO3- 3.607e-003 3.340e-003 -2.443 -2.476 -0.033

CO2 5.790e-004 5.798e-004 -3.237 -3.237 0.001

CaHCO3+ 3.804e-005 3.523e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.397e-005 -4.821 -4.855 -0.034

CaCO3 2.673e-006 2.677e-006 -5.573 -5.572 0.001

CO3-2 2.606e-006 1.917e-006 -5.584 -5.717 -0.133

MgCO3 5.979e-007 5.987e-007 -6.223 -6.223 0.001

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaCO3- 2.420e-010 2.236e-010 -9.616 -9.650 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.456e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.804e-005 3.523e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.673e-006 2.677e-006 -5.573 -5.572 0.001

CaOH+ 2.454e-009 2.268e-009 -8.610 -8.644 -0.034

CaHSO4+ 5.061e-012 4.677e-012 -11.296 -11.330 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 7.307e-026

H2 3.653e-026 3.658e-026 -25.437 -25.437 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.536e-013 1.538e-013 -12.814 -12.813 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.397e-005 -4.821 -4.855 -0.034

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 5.979e-007 5.987e-007 -6.223 -6.223 0.001

MgOH+ 1.041e-008 9.621e-009 -7.983 -8.017 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

NaCO3- 2.420e-010 2.236e-010 -9.616 -9.650 -0.034

NaOH 8.807e-013 8.819e-013 -12.055 -12.055 0.001

O(0) 3.757e-004

O2 1.879e-004 1.881e-004 -3.726 -3.726 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.452e-010 4.114e-010 -9.351 -9.386 -0.034

CaHSO4+ 5.061e-012 4.677e-012 -11.296 -11.330 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.45 -8.74 -8.29 CaCO3

Calcite -0.30 -8.74 -8.44 CaCO3

CO2(g) -1.86 -3.24 -1.37 CO2

Dolomite -0.98 -17.89 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.32 -25.44 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.73 -2.83 O2

Initial solution 42. 29/8/2012 22:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.745e-004 3.745e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.193e-003

Total CO2 (mol/kg) = 4.193e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0256 0.8088

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.524e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.193e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.279e-004 5.286e-004 -3.277 -3.277 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CO3-2 2.856e-006 2.101e-006 -5.544 -5.678 -0.133

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.930e-006 2.934e-006 -5.533 -5.533 0.001

CaOH+ 2.691e-009 2.486e-009 -8.570 -8.604 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.553e-007 6.562e-007 -6.184 -6.183 0.001

MgOH+ 1.141e-008 1.055e-008 -7.943 -7.977 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.653e-010 2.451e-010 -9.576 -9.611 -0.034

NaOH 9.657e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 3.745e-004

O2 1.872e-004 1.875e-004 -3.728 -3.727 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.061e-010 3.752e-010 -9.391 -9.426 -0.034

CaHSO4+ 4.615e-012 4.265e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.73 -2.83 O2

Initial solution 43. 29/8/2012 22:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.045e-004 4.045e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99896

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.147e-003

Total CO2 (mol/kg) = 4.147e-003

Temperature (deg C) = 17.400

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0027 0.8072

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.036e-007 9.560e-008 -6.985 -7.020 -0.035

H+ 6.179e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.147e-003

HCO3- 3.605e-003 3.338e-003 -2.443 -2.476 -0.033

CO2 4.822e-004 4.828e-004 -3.317 -3.316 0.001

CaHCO3+ 3.793e-005 3.513e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.510e-005 1.395e-005 -4.821 -4.855 -0.034

CaCO3 3.199e-006 3.203e-006 -5.495 -5.494 0.001

CO3-2 3.123e-006 2.298e-006 -5.505 -5.639 -0.133

MgCO3 7.155e-007 7.164e-007 -6.145 -6.145 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.885e-010 2.666e-010 -9.540 -9.574 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.793e-005 3.513e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.199e-006 3.203e-006 -5.495 -5.494 0.001

CaOH+ 2.950e-009 2.726e-009 -8.530 -8.564 -0.034

CaHSO4+ 4.202e-012 3.883e-012 -11.377 -11.411 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.060e-026

H2 2.530e-026 2.534e-026 -25.597 -25.596 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.395e-005 -4.821 -4.855 -0.034

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

MgCO3 7.155e-007 7.164e-007 -6.145 -6.145 0.001

MgOH+ 1.240e-008 1.146e-008 -7.907 -7.941 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.885e-010 2.666e-010 -9.540 -9.574 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 4.045e-004

O2 2.023e-004 2.025e-004 -3.694 -3.694 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

HSO4- 3.697e-010 3.416e-010 -9.432 -9.466 -0.034

CaHSO4+ 4.202e-012 3.883e-012 -11.377 -11.411 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.37 CO2

Dolomite -0.83 -17.74 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.69 -2.83 O2

Initial solution 44. 29/8/2012 22:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.801e-004 3.801e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.130

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.634e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.287e-003

Total CO2 (mol/kg) = 4.287e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551930e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0972 0.8130

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.106e-008 7.482e-008 -7.091 -7.126 -0.035

H+ 7.960e-008 7.413e-008 -7.099 -7.130 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.287e-003

HCO3- 3.608e-003 3.341e-003 -2.443 -2.476 -0.033

CO2 6.206e-004 6.214e-004 -3.207 -3.207 0.001

CaHCO3+ 3.805e-005 3.524e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.512e-005 1.397e-005 -4.821 -4.855 -0.034

CaCO3 2.496e-006 2.499e-006 -5.603 -5.602 0.001

CO3-2 2.433e-006 1.789e-006 -5.614 -5.747 -0.133

MgCO3 5.582e-007 5.589e-007 -6.253 -6.253 0.001

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaCO3- 2.259e-010 2.087e-010 -9.646 -9.680 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.457e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.805e-005 3.524e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

CaCO3 2.496e-006 2.499e-006 -5.603 -5.602 0.001

CaOH+ 2.291e-009 2.117e-009 -8.640 -8.674 -0.034

CaHSO4+ 5.424e-012 5.012e-012 -11.266 -11.300 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 8.390e-026

H2 4.195e-026 4.200e-026 -25.377 -25.377 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.433e-013 1.435e-013 -12.844 -12.843 0.001

Mg 5.184e-004

Mg+2 4.977e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.512e-005 1.397e-005 -4.821 -4.855 -0.034

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 5.582e-007 5.589e-007 -6.253 -6.253 0.001

MgOH+ 9.716e-009 8.979e-009 -8.012 -8.047 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

NaCO3- 2.259e-010 2.087e-010 -9.646 -9.680 -0.034

NaOH 8.219e-013 8.230e-013 -12.085 -12.085 0.001

O(0) 3.801e-004

O2 1.901e-004 1.903e-004 -3.721 -3.721 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.770e-010 4.408e-010 -9.321 -9.356 -0.034

CaHSO4+ 5.424e-012 5.012e-012 -11.266 -11.300 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.48 -8.77 -8.29 CaCO3

Calcite -0.33 -8.77 -8.44 CaCO3

CO2(g) -1.83 -3.21 -1.37 CO2

Dolomite -1.04 -17.95 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.26 -25.38 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 45. 29/8/2012 22:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.770e-004 3.770e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551906e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0063 0.8077

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.770e-004

O2 1.885e-004 1.887e-004 -3.725 -3.724 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 46. 29/8/2012 23:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.776e-004 3.776e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99896

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.170e-003

Total CO2 (mol/kg) = 4.170e-003

Temperature (deg C) = 17.400

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551906e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0152 0.8080

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.891e-008 9.130e-008 -7.005 -7.040 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.170e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.050e-004 5.056e-004 -3.297 -3.296 0.001

CaHCO3+ 3.794e-005 3.513e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.056e-006 3.060e-006 -5.515 -5.514 0.001

CO3-2 2.983e-006 2.195e-006 -5.525 -5.659 -0.133

MgCO3 6.834e-007 6.843e-007 -6.165 -6.165 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.756e-010 2.547e-010 -9.560 -9.594 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.794e-005 3.513e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.056e-006 3.060e-006 -5.515 -5.514 0.001

CaOH+ 2.818e-009 2.604e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.400e-012 4.066e-012 -11.357 -11.391 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.549e-026

H2 2.774e-026 2.778e-026 -25.557 -25.556 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

MgCO3 6.834e-007 6.843e-007 -6.165 -6.165 0.001

MgOH+ 1.184e-008 1.094e-008 -7.927 -7.961 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.756e-010 2.547e-010 -9.560 -9.594 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.776e-004

O2 1.888e-004 1.891e-004 -3.724 -3.723 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

HSO4- 3.871e-010 3.577e-010 -9.412 -9.446 -0.034

CaHSO4+ 4.400e-012 4.066e-012 -11.357 -11.391 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.87 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 47. 29/8/2012 23:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.101e-004 4.101e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551909e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0155 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.101e-004

O2 2.051e-004 2.053e-004 -3.688 -3.688 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.69 -2.83 O2

Initial solution 48. 29/8/2012 23:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.245e-004 4.245e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99896

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.182e-003

Total CO2 (mol/kg) = 4.182e-003

Temperature (deg C) = 17.400

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551913e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0380 0.8093

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.666e-008 8.922e-008 -7.015 -7.050 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.182e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.168e-004 5.174e-004 -3.287 -3.286 0.001

CaHCO3+ 3.794e-005 3.514e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.987e-006 2.991e-006 -5.525 -5.524 0.001

CO3-2 2.916e-006 2.145e-006 -5.535 -5.669 -0.133

MgCO3 6.680e-007 6.688e-007 -6.175 -6.175 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.693e-010 2.489e-010 -9.570 -9.604 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.794e-005 3.514e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 2.987e-006 2.991e-006 -5.525 -5.524 0.001

CaOH+ 2.753e-009 2.545e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.503e-012 4.161e-012 -11.347 -11.381 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.810e-026

H2 2.905e-026 2.909e-026 -25.537 -25.536 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

MgCO3 6.680e-007 6.688e-007 -6.175 -6.175 0.001

MgOH+ 1.157e-008 1.069e-008 -7.937 -7.971 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.693e-010 2.489e-010 -9.570 -9.604 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 4.245e-004

O2 2.123e-004 2.125e-004 -3.673 -3.673 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

HSO4- 3.961e-010 3.660e-010 -9.402 -9.436 -0.034

CaHSO4+ 4.503e-012 4.161e-012 -11.347 -11.381 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.89 -17.80 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.67 -2.83 O2

Initial solution 49. 29/8/2012 23:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.026e-004 4.026e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551908e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0135 0.8081

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.026e-004

O2 2.013e-004 2.016e-004 -3.696 -3.696 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 50. 30/8/2012 00:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.408e-004 4.408e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99896

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.182e-003

Total CO2 (mol/kg) = 4.182e-003

Temperature (deg C) = 17.400

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551915e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0420 0.8095

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.666e-008 8.922e-008 -7.015 -7.050 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.182e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.168e-004 5.174e-004 -3.287 -3.286 0.001

CaHCO3+ 3.794e-005 3.514e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.987e-006 2.991e-006 -5.525 -5.524 0.001

CO3-2 2.916e-006 2.145e-006 -5.535 -5.669 -0.133

MgCO3 6.680e-007 6.688e-007 -6.175 -6.175 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.693e-010 2.489e-010 -9.570 -9.604 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.794e-005 3.514e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 2.987e-006 2.991e-006 -5.525 -5.524 0.001

CaOH+ 2.753e-009 2.545e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.503e-012 4.161e-012 -11.347 -11.381 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.810e-026

H2 2.905e-026 2.909e-026 -25.537 -25.536 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

MgCO3 6.680e-007 6.688e-007 -6.175 -6.175 0.001

MgOH+ 1.157e-008 1.069e-008 -7.937 -7.971 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.693e-010 2.489e-010 -9.570 -9.604 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 4.408e-004

O2 2.204e-004 2.207e-004 -3.657 -3.656 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

HSO4- 3.961e-010 3.660e-010 -9.402 -9.436 -0.034

CaHSO4+ 4.503e-012 4.161e-012 -11.347 -11.381 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.89 -17.80 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.82 -3.66 -2.83 O2

Initial solution 51. 30/8/2012 00:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.707e-004 3.707e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551908e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0145 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.159e-004 5.165e-004 -3.287 -3.287 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CO3-2 2.923e-006 2.150e-006 -5.534 -5.668 -0.133

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CaOH+ 2.753e-009 2.544e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 3.707e-004

O2 1.854e-004 1.856e-004 -3.732 -3.731 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.968e-010 3.667e-010 -9.401 -9.436 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.90 -3.73 -2.83 O2

Initial solution 52. 30/8/2012 00:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.714e-004 3.714e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551908e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0147 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.159e-004 5.165e-004 -3.287 -3.287 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CO3-2 2.923e-006 2.150e-006 -5.534 -5.668 -0.133

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CaOH+ 2.753e-009 2.544e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 3.714e-004

O2 1.857e-004 1.859e-004 -3.731 -3.731 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.968e-010 3.667e-010 -9.401 -9.436 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.90 -3.73 -2.83 O2

Initial solution 53. 30/8/2012 00:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.214e-004 4.214e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99896

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.182e-003

Total CO2 (mol/kg) = 4.182e-003

Temperature (deg C) = 17.400

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551913e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0372 0.8092

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.666e-008 8.922e-008 -7.015 -7.050 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.182e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.168e-004 5.174e-004 -3.287 -3.286 0.001

CaHCO3+ 3.794e-005 3.514e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.987e-006 2.991e-006 -5.525 -5.524 0.001

CO3-2 2.916e-006 2.145e-006 -5.535 -5.669 -0.133

MgCO3 6.680e-007 6.688e-007 -6.175 -6.175 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.693e-010 2.489e-010 -9.570 -9.604 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.794e-005 3.514e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 2.987e-006 2.991e-006 -5.525 -5.524 0.001

CaOH+ 2.753e-009 2.545e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.503e-012 4.161e-012 -11.347 -11.381 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.810e-026

H2 2.905e-026 2.909e-026 -25.537 -25.536 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

MgCO3 6.680e-007 6.688e-007 -6.175 -6.175 0.001

MgOH+ 1.157e-008 1.069e-008 -7.937 -7.971 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.693e-010 2.489e-010 -9.570 -9.604 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 4.214e-004

O2 2.107e-004 2.110e-004 -3.676 -3.676 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

HSO4- 3.961e-010 3.660e-010 -9.402 -9.436 -0.034

CaHSO4+ 4.503e-012 4.161e-012 -11.347 -11.381 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.89 -17.80 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.68 -2.83 O2

Initial solution 54. 30/8/2012 01:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.945e-004 3.945e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551908e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0113 0.8080

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.945e-004

O2 1.972e-004 1.975e-004 -3.705 -3.704 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.70 -2.83 O2

Initial solution 55. 30/8/2012 01:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.782e-004 3.782e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551908e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0167 0.8083

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.159e-004 5.165e-004 -3.287 -3.287 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CO3-2 2.923e-006 2.150e-006 -5.534 -5.668 -0.133

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CaOH+ 2.753e-009 2.544e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 3.782e-004

O2 1.891e-004 1.894e-004 -3.723 -3.723 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.968e-010 3.667e-010 -9.401 -9.436 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 56. 30/8/2012 01:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.139e-004 4.139e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551910e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0165 0.8083

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.139e-004

O2 2.069e-004 2.072e-004 -3.684 -3.684 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.68 -2.83 O2

Initial solution 57. 30/8/2012 01:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.857e-004 3.857e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551909e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0188 0.8084

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.159e-004 5.165e-004 -3.287 -3.287 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CO3-2 2.923e-006 2.150e-006 -5.534 -5.668 -0.133

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CaOH+ 2.753e-009 2.544e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 3.857e-004

O2 1.929e-004 1.931e-004 -3.715 -3.714 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.968e-010 3.667e-010 -9.401 -9.436 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 58. 30/8/2012 02:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.714e-004 3.714e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0047 0.8076

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.714e-004

O2 1.857e-004 1.859e-004 -3.731 -3.731 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.90 -3.73 -2.83 O2

Initial solution 59. 30/8/2012 02:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.220e-004 4.220e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99896

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.170e-003

Total CO2 (mol/kg) = 4.170e-003

Temperature (deg C) = 17.400

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0273 0.8086

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.891e-008 9.130e-008 -7.005 -7.040 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.170e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.050e-004 5.056e-004 -3.297 -3.296 0.001

CaHCO3+ 3.794e-005 3.513e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.056e-006 3.060e-006 -5.515 -5.514 0.001

CO3-2 2.983e-006 2.195e-006 -5.525 -5.659 -0.133

MgCO3 6.835e-007 6.843e-007 -6.165 -6.165 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.756e-010 2.547e-010 -9.560 -9.594 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.794e-005 3.513e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.056e-006 3.060e-006 -5.515 -5.514 0.001

CaOH+ 2.818e-009 2.604e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.400e-012 4.066e-012 -11.357 -11.391 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.549e-026

H2 2.774e-026 2.778e-026 -25.557 -25.556 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

MgCO3 6.835e-007 6.843e-007 -6.165 -6.165 0.001

MgOH+ 1.184e-008 1.094e-008 -7.927 -7.961 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.756e-010 2.547e-010 -9.560 -9.594 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.220e-004

O2 2.110e-004 2.113e-004 -3.676 -3.675 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

HSO4- 3.871e-010 3.577e-010 -9.412 -9.446 -0.034

CaHSO4+ 4.400e-012 4.066e-012 -11.357 -11.391 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.87 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.68 -2.83 O2

Initial solution 60. 30/8/2012 02:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.245e-004 4.245e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551913e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0292 0.8090

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.159e-004 5.165e-004 -3.287 -3.287 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CO3-2 2.923e-006 2.150e-006 -5.534 -5.668 -0.133

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 2.998e-006 3.002e-006 -5.523 -5.523 0.001

CaOH+ 2.753e-009 2.544e-009 -8.560 -8.594 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.723e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.705e-007 6.714e-007 -6.174 -6.173 0.001

MgOH+ 1.168e-008 1.079e-008 -7.933 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.714e-010 2.508e-010 -9.566 -9.601 -0.034

NaOH 9.882e-013 9.895e-013 -12.005 -12.005 0.001

O(0) 4.245e-004

O2 2.123e-004 2.125e-004 -3.673 -3.673 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.968e-010 3.667e-010 -9.401 -9.436 -0.034

CaHSO4+ 4.510e-012 4.168e-012 -11.346 -11.380 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.88 -17.79 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.67 -2.83 O2

Initial solution 61. 30/8/2012 02:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.820e-004 3.820e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99896

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.170e-003

Total CO2 (mol/kg) = 4.170e-003

Temperature (deg C) = 17.400

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551907e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0165 0.8080

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.891e-008 9.130e-008 -7.005 -7.040 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.170e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.050e-004 5.056e-004 -3.297 -3.296 0.001

CaHCO3+ 3.794e-005 3.513e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.056e-006 3.060e-006 -5.515 -5.514 0.001

CO3-2 2.983e-006 2.195e-006 -5.525 -5.659 -0.133

MgCO3 6.834e-007 6.843e-007 -6.165 -6.165 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.756e-010 2.547e-010 -9.560 -9.594 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.794e-005 3.513e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.056e-006 3.060e-006 -5.515 -5.514 0.001

CaOH+ 2.818e-009 2.604e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.400e-012 4.066e-012 -11.357 -11.391 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.549e-026

H2 2.774e-026 2.778e-026 -25.557 -25.556 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

MgCO3 6.834e-007 6.843e-007 -6.165 -6.165 0.001

MgOH+ 1.184e-008 1.094e-008 -7.927 -7.961 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.756e-010 2.547e-010 -9.560 -9.594 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.820e-004

O2 1.910e-004 1.912e-004 -3.719 -3.718 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

HSO4- 3.871e-010 3.577e-010 -9.412 -9.446 -0.034

CaHSO4+ 4.400e-012 4.066e-012 -11.357 -11.391 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.87 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 62. 30/8/2012 03:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.826e-004 3.826e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99896

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.170e-003

Total CO2 (mol/kg) = 4.170e-003

Temperature (deg C) = 17.400

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551907e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0167 0.8080

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.891e-008 9.130e-008 -7.005 -7.040 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.170e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.050e-004 5.056e-004 -3.297 -3.296 0.001

CaHCO3+ 3.794e-005 3.513e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.056e-006 3.060e-006 -5.515 -5.514 0.001

CO3-2 2.983e-006 2.195e-006 -5.525 -5.659 -0.133

MgCO3 6.834e-007 6.843e-007 -6.165 -6.165 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.756e-010 2.547e-010 -9.560 -9.594 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.455e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.794e-005 3.513e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.056e-006 3.060e-006 -5.515 -5.514 0.001

CaOH+ 2.818e-009 2.604e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.400e-012 4.066e-012 -11.357 -11.391 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.549e-026

H2 2.774e-026 2.778e-026 -25.557 -25.556 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

MgCO3 6.834e-007 6.843e-007 -6.165 -6.165 0.001

MgOH+ 1.184e-008 1.094e-008 -7.927 -7.961 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

NaCO3- 2.756e-010 2.547e-010 -9.560 -9.594 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.826e-004

O2 1.913e-004 1.916e-004 -3.718 -3.718 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.042e-006 5.049e-006 -5.297 -5.297 0.001

NaSO4- 3.418e-009 3.158e-009 -8.466 -8.501 -0.034

KSO4- 1.460e-009 1.349e-009 -8.836 -8.870 -0.034

HSO4- 3.871e-010 3.577e-010 -9.412 -9.446 -0.034

CaHSO4+ 4.400e-012 4.066e-012 -11.357 -11.391 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.87 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.72 -2.83 O2

Initial solution 63. 30/8/2012 03:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.089e-004 4.089e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551909e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0152 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.089e-004

O2 2.044e-004 2.047e-004 -3.689 -3.689 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.69 -2.83 O2

Initial solution 64. 30/8/2012 03:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.814e-004 3.814e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.140

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.634e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.273e-003

Total CO2 (mol/kg) = 4.273e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551927e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0876 0.8124

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.295e-008 7.656e-008 -7.081 -7.116 -0.035

H+ 7.779e-008 7.244e-008 -7.109 -7.140 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.273e-003

HCO3- 3.608e-003 3.341e-003 -2.443 -2.476 -0.033

CO2 6.064e-004 6.072e-004 -3.217 -3.217 0.001

CaHCO3+ 3.805e-005 3.524e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.512e-005 1.397e-005 -4.821 -4.855 -0.034

CaCO3 2.554e-006 2.557e-006 -5.593 -5.592 0.001

CO3-2 2.489e-006 1.831e-006 -5.604 -5.737 -0.133

MgCO3 5.711e-007 5.719e-007 -6.243 -6.243 0.001

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaCO3- 2.311e-010 2.136e-010 -9.636 -9.670 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.457e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.805e-005 3.524e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

CaCO3 2.554e-006 2.557e-006 -5.593 -5.592 0.001

CaOH+ 2.344e-009 2.166e-009 -8.630 -8.664 -0.034

CaHSO4+ 5.300e-012 4.898e-012 -11.276 -11.310 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 8.012e-026

H2 4.006e-026 4.011e-026 -25.397 -25.397 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.467e-013 1.469e-013 -12.834 -12.833 0.001

Mg 5.184e-004

Mg+2 4.977e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.512e-005 1.397e-005 -4.821 -4.855 -0.034

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 5.711e-007 5.719e-007 -6.243 -6.243 0.001

MgOH+ 9.943e-009 9.188e-009 -8.003 -8.037 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.733e-008 1.735e-008 -7.761 -7.761 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

NaCO3- 2.311e-010 2.136e-010 -9.636 -9.670 -0.034

NaOH 8.411e-013 8.422e-013 -12.075 -12.075 0.001

O(0) 3.814e-004

O2 1.907e-004 1.909e-004 -3.720 -3.719 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.167e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

MgSO4 5.055e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.159e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 4.662e-010 4.308e-010 -9.331 -9.366 -0.034

CaHSO4+ 5.300e-012 4.898e-012 -11.276 -11.310 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.47 -8.76 -8.29 CaCO3

Calcite -0.32 -8.76 -8.44 CaCO3

CO2(g) -1.84 -3.22 -1.37 CO2

Dolomite -1.02 -17.93 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.28 -25.40 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 65. 30/8/2012 03:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.045e-004 4.045e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.158e-003

Total CO2 (mol/kg) = 4.158e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0140 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.158e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.027e-004 5.034e-004 -3.299 -3.298 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.051e-006 3.055e-006 -5.516 -5.515 0.001

CO3-2 2.982e-006 2.194e-006 -5.526 -5.659 -0.133

MgCO3 6.845e-007 6.854e-007 -6.165 -6.164 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.770e-010 2.560e-010 -9.558 -9.592 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.051e-006 3.055e-006 -5.516 -5.515 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.399e-012 4.065e-012 -11.357 -11.391 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 6.845e-007 6.854e-007 -6.165 -6.164 0.001

MgOH+ 1.195e-008 1.105e-008 -7.922 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.770e-010 2.560e-010 -9.558 -9.592 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.045e-004

O2 2.023e-004 2.025e-004 -3.694 -3.694 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.879e-010 3.585e-010 -9.411 -9.445 -0.034

CaHSO4+ 4.399e-012 4.065e-012 -11.357 -11.391 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.87 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.69 -2.83 O2

Initial solution 66. 30/8/2012 04:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.064e-004 4.064e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551909e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0145 0.8082

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.064e-004

O2 2.032e-004 2.035e-004 -3.692 -3.692 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.69 -2.83 O2

Initial solution 67. 30/8/2012 04:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.270e-004 4.270e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0199 0.8085

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.270e-004

O2 2.135e-004 2.138e-004 -3.671 -3.670 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.67 -2.83 O2

Initial solution 68. 30/8/2012 04:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.314e-004 4.314e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0210 0.8086

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.041e-004 5.047e-004 -3.297 -3.297 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CO3-2 2.991e-006 2.200e-006 -5.524 -5.658 -0.133

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.454e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.067e-006 3.071e-006 -5.513 -5.513 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.584 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 6.861e-007 6.870e-007 -6.164 -6.163 0.001

MgOH+ 1.195e-008 1.104e-008 -7.923 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.777e-010 2.566e-010 -9.556 -9.591 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.314e-004

O2 2.157e-004 2.160e-004 -3.666 -3.666 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.878e-010 3.584e-010 -9.411 -9.446 -0.034

CaHSO4+ 4.407e-012 4.073e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.83 -3.67 -2.83 O2

Initial solution 69. 30/8/2012 04:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.007e-004 4.007e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.158e-003

Total CO2 (mol/kg) = 4.158e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551906e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0030 0.8075

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.158e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 4.926e-004 4.932e-004 -3.308 -3.307 0.001

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.138e-006 3.142e-006 -5.503 -5.503 0.001

CO3-2 3.060e-006 2.251e-006 -5.514 -5.648 -0.133

MgCO3 7.020e-007 7.029e-007 -6.154 -6.153 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.842e-010 2.626e-010 -9.546 -9.581 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.453e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.801e-005 3.520e-005 -4.420 -4.453 -0.033

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.138e-006 3.142e-006 -5.503 -5.503 0.001

CaOH+ 2.883e-009 2.664e-009 -8.540 -8.574 -0.034

CaHSO4+ 4.307e-012 3.980e-012 -11.366 -11.400 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 7.020e-007 7.029e-007 -6.154 -6.153 0.001

MgOH+ 1.223e-008 1.130e-008 -7.913 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.842e-010 2.626e-010 -9.546 -9.581 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.007e-004

O2 2.004e-004 2.006e-004 -3.698 -3.698 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.351e-009 -8.835 -8.869 -0.034

HSO4- 3.790e-010 3.502e-010 -9.421 -9.456 -0.034

CaHSO4+ 4.307e-012 3.980e-012 -11.366 -11.400 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.84 -17.75 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 70. 30/8/2012 05:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.870e-004 3.870e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.170

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.622e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.220e-003

Total CO2 (mol/kg) = 4.220e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551916e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0592 0.8108

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.887e-008 8.204e-008 -7.051 -7.086 -0.035

H+ 7.259e-008 6.761e-008 -7.139 -7.170 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.220e-003

HCO3- 3.597e-003 3.331e-003 -2.444 -2.477 -0.033

CO2 5.643e-004 5.650e-004 -3.248 -3.248 0.001

CaHCO3+ 3.784e-005 3.504e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.508e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 2.721e-006 2.725e-006 -5.565 -5.565 0.001

CO3-2 2.658e-006 1.956e-006 -5.575 -5.709 -0.133

MgCO3 6.103e-007 6.111e-007 -6.214 -6.214 0.001

NaHCO3 1.728e-008 1.730e-008 -7.762 -7.762 0.001

NaCO3- 2.469e-010 2.282e-010 -9.607 -9.642 -0.034

Ca 1.336e-003

Ca+2 1.283e-003 9.433e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.784e-005 3.504e-005 -4.422 -4.455 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 2.721e-006 2.725e-006 -5.565 -5.565 0.001

CaOH+ 2.505e-009 2.315e-009 -8.601 -8.635 -0.034

CaHSO4+ 4.936e-012 4.562e-012 -11.307 -11.341 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.978e-026

H2 3.489e-026 3.494e-026 -25.457 -25.457 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.572e-013 1.574e-013 -12.804 -12.803 0.001

Mg 5.184e-004

Mg+2 4.977e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.508e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 6.103e-007 6.111e-007 -6.214 -6.214 0.001

MgOH+ 1.066e-008 9.848e-009 -7.972 -8.007 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.728e-008 1.730e-008 -7.762 -7.762 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.469e-010 2.282e-010 -9.607 -9.642 -0.034

NaOH 9.013e-013 9.025e-013 -12.045 -12.045 0.001

O(0) 3.870e-004

O2 1.935e-004 1.937e-004 -3.713 -3.713 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 4.353e-010 4.023e-010 -9.361 -9.395 -0.034

CaHSO4+ 4.936e-012 4.562e-012 -11.307 -11.341 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.44 -8.73 -8.29 CaCO3

Calcite -0.29 -8.73 -8.44 CaCO3

CO2(g) -1.87 -3.25 -1.37 CO2

Dolomite -0.97 -17.88 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.34 -25.46 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 71. 30/8/2012 05:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.020e-004 4.020e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.182e-003

Total CO2 (mol/kg) = 4.182e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551910e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0333 0.8093

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.523e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.182e-003

HCO3- 3.596e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.265e-004 5.272e-004 -3.279 -3.278 0.001

CaHCO3+ 3.782e-005 3.503e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 2.915e-006 2.919e-006 -5.535 -5.535 0.001

CO3-2 2.848e-006 2.096e-006 -5.545 -5.679 -0.133

MgCO3 6.538e-007 6.546e-007 -6.185 -6.184 0.001

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaCO3- 2.645e-010 2.445e-010 -9.578 -9.612 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.431e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.782e-005 3.503e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 2.915e-006 2.919e-006 -5.535 -5.535 0.001

CaOH+ 2.684e-009 2.480e-009 -8.571 -8.605 -0.034

CaHSO4+ 4.606e-012 4.257e-012 -11.337 -11.371 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.687e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 6.538e-007 6.546e-007 -6.185 -6.184 0.001

MgOH+ 1.142e-008 1.055e-008 -7.942 -7.977 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.645e-010 2.445e-010 -9.578 -9.612 -0.034

NaOH 9.658e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 4.020e-004

O2 2.010e-004 2.013e-004 -3.697 -3.696 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 4.062e-010 3.754e-010 -9.391 -9.425 -0.034

CaHSO4+ 4.606e-012 4.257e-012 -11.337 -11.371 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.91 -17.82 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 72. 30/8/2012 05:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.007e-004 4.007e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.160

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.622e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.233e-003

Total CO2 (mol/kg) = 4.233e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551920e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0730 0.8116

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.685e-008 8.017e-008 -7.061 -7.096 -0.035

H+ 7.428e-008 6.918e-008 -7.129 -7.160 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.233e-003

HCO3- 3.597e-003 3.331e-003 -2.444 -2.477 -0.033

CO2 5.775e-004 5.782e-004 -3.238 -3.238 0.001

CaHCO3+ 3.784e-005 3.505e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.508e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 2.660e-006 2.663e-006 -5.575 -5.575 0.001

CO3-2 2.598e-006 1.912e-006 -5.585 -5.719 -0.133

MgCO3 5.965e-007 5.973e-007 -6.224 -6.224 0.001

NaHCO3 1.728e-008 1.730e-008 -7.762 -7.762 0.001

NaCO3- 2.413e-010 2.230e-010 -9.617 -9.652 -0.034

Ca 1.336e-003

Ca+2 1.283e-003 9.433e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.784e-005 3.505e-005 -4.422 -4.455 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 2.660e-006 2.663e-006 -5.575 -5.575 0.001

CaOH+ 2.448e-009 2.263e-009 -8.611 -8.645 -0.034

CaHSO4+ 5.051e-012 4.668e-012 -11.297 -11.331 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 7.307e-026

H2 3.653e-026 3.658e-026 -25.437 -25.437 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.536e-013 1.538e-013 -12.814 -12.813 0.001

Mg 5.184e-004

Mg+2 4.977e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.508e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.059e-006 5.066e-006 -5.296 -5.295 0.001

MgCO3 5.965e-007 5.973e-007 -6.224 -6.224 0.001

MgOH+ 1.041e-008 9.624e-009 -7.982 -8.017 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.728e-008 1.730e-008 -7.762 -7.762 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.413e-010 2.230e-010 -9.617 -9.652 -0.034

NaOH 8.808e-013 8.819e-013 -12.055 -12.055 0.001

O(0) 4.007e-004

O2 2.004e-004 2.006e-004 -3.698 -3.698 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.059e-006 5.066e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 4.454e-010 4.116e-010 -9.351 -9.385 -0.034

CaHSO4+ 5.051e-012 4.668e-012 -11.297 -11.331 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.45 -8.74 -8.29 CaCO3

Calcite -0.30 -8.74 -8.44 CaCO3

CO2(g) -1.86 -3.24 -1.37 CO2

Dolomite -0.99 -17.90 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.32 -25.44 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 73. 30/8/2012 05:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.020e-004 4.020e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.250

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.123e-003

Total CO2 (mol/kg) = 4.123e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551898e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9833 0.8064

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.068e-007 9.863e-008 -6.971 -7.006 -0.035

H+ 6.038e-008 5.623e-008 -7.219 -7.250 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.123e-003

HCO3- 3.594e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.690e-004 4.697e-004 -3.329 -3.328 0.001

CaHCO3+ 3.780e-005 3.501e-005 -4.423 -4.456 -0.033

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.268e-006 3.273e-006 -5.486 -5.485 0.001

CO3-2 3.194e-006 2.350e-006 -5.496 -5.629 -0.133

MgCO3 7.332e-007 7.341e-007 -6.135 -6.134 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.967e-010 2.742e-010 -9.528 -9.562 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.780e-005 3.501e-005 -4.423 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.268e-006 3.273e-006 -5.486 -5.485 0.001

CaOH+ 3.011e-009 2.782e-009 -8.521 -8.556 -0.034

CaHSO4+ 4.104e-012 3.793e-012 -11.387 -11.421 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 4.828e-026

H2 2.414e-026 2.417e-026 -25.617 -25.617 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.890e-013 1.892e-013 -12.724 -12.723 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.332e-007 7.341e-007 -6.135 -6.134 0.001

MgOH+ 1.281e-008 1.184e-008 -7.892 -7.927 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.967e-010 2.742e-010 -9.528 -9.562 -0.034

NaOH 1.084e-012 1.085e-012 -11.965 -11.965 0.001

O(0) 4.020e-004

O2 2.010e-004 2.013e-004 -3.697 -3.696 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.621e-010 3.346e-010 -9.441 -9.475 -0.034

CaHSO4+ 4.104e-012 3.793e-012 -11.387 -11.421 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.36 -8.65 -8.29 CaCO3

Calcite -0.21 -8.65 -8.44 CaCO3

CO2(g) -1.95 -3.33 -1.37 CO2

Dolomite -0.81 -17.72 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.50 -25.62 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 74. 30/8/2012 06:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.189e-004 4.189e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9978 0.8072

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.044e-007 9.639e-008 -6.981 -7.016 -0.035

H+ 6.179e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.605e-003 3.338e-003 -2.443 -2.476 -0.033

CO2 4.813e-004 4.819e-004 -3.318 -3.317 0.001

CaHCO3+ 3.800e-005 3.519e-005 -4.420 -4.454 -0.033

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.211e-006 3.215e-006 -5.493 -5.493 0.001

CO3-2 3.131e-006 2.303e-006 -5.504 -5.638 -0.133

MgCO3 7.183e-007 7.192e-007 -6.144 -6.143 0.001

NaHCO3 1.731e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.908e-010 2.687e-010 -9.536 -9.571 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.453e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.800e-005 3.519e-005 -4.420 -4.454 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.211e-006 3.215e-006 -5.493 -5.493 0.001

CaOH+ 2.950e-009 2.726e-009 -8.530 -8.564 -0.034

CaHSO4+ 4.209e-012 3.889e-012 -11.376 -11.410 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.055e-026

H2 2.528e-026 2.531e-026 -25.597 -25.597 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.462e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.510e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

MgCO3 7.183e-007 7.192e-007 -6.144 -6.143 0.001

MgOH+ 1.251e-008 1.156e-008 -7.903 -7.937 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.731e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

NaCO3- 2.908e-010 2.687e-010 -9.536 -9.571 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 4.189e-004

O2 2.094e-004 2.097e-004 -3.679 -3.678 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.054e-006 5.061e-006 -5.296 -5.296 0.001

NaSO4- 3.419e-009 3.160e-009 -8.466 -8.500 -0.034

KSO4- 1.462e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.703e-010 3.422e-010 -9.431 -9.466 -0.034

CaHSO4+ 4.209e-012 3.889e-012 -11.376 -11.410 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.37 CO2

Dolomite -0.82 -17.73 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.84 -3.68 -2.83 O2

Initial solution 75. 30/8/2012 06:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.957e-004 3.957e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.158e-003

Total CO2 (mol/kg) = 4.158e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0116 0.8080

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.158e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.027e-004 5.034e-004 -3.299 -3.298 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.051e-006 3.055e-006 -5.516 -5.515 0.001

CO3-2 2.982e-006 2.194e-006 -5.526 -5.659 -0.133

MgCO3 6.845e-007 6.854e-007 -6.165 -6.164 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.770e-010 2.560e-010 -9.558 -9.592 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.051e-006 3.055e-006 -5.516 -5.515 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.399e-012 4.065e-012 -11.357 -11.391 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 6.845e-007 6.854e-007 -6.165 -6.164 0.001

MgOH+ 1.195e-008 1.105e-008 -7.922 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.770e-010 2.560e-010 -9.558 -9.592 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.957e-004

O2 1.979e-004 1.981e-004 -3.704 -3.703 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.879e-010 3.585e-010 -9.411 -9.445 -0.034

CaHSO4+ 4.399e-012 4.065e-012 -11.357 -11.391 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.87 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.70 -2.83 O2

Initial solution 76. 30/8/2012 06:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.151e-004 4.151e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.135e-003

Total CO2 (mol/kg) = 4.135e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551902e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9968 0.8072

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.044e-007 9.639e-008 -6.981 -7.016 -0.035

H+ 6.179e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.135e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.800e-004 4.806e-004 -3.319 -3.318 0.001

CaHCO3+ 3.780e-005 3.501e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.194e-006 3.198e-006 -5.496 -5.495 0.001

CO3-2 3.122e-006 2.297e-006 -5.506 -5.639 -0.133

MgCO3 7.166e-007 7.175e-007 -6.145 -6.144 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.780e-005 3.501e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.194e-006 3.198e-006 -5.496 -5.495 0.001

CaOH+ 2.942e-009 2.719e-009 -8.531 -8.566 -0.034

CaHSO4+ 4.200e-012 3.882e-012 -11.377 -11.411 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.055e-026

H2 2.528e-026 2.531e-026 -25.597 -25.597 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.166e-007 7.175e-007 -6.145 -6.144 0.001

MgOH+ 1.252e-008 1.157e-008 -7.902 -7.937 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 4.151e-004

O2 2.076e-004 2.078e-004 -3.683 -3.682 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.705e-010 3.424e-010 -9.431 -9.465 -0.034

CaHSO4+ 4.200e-012 3.882e-012 -11.377 -11.411 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.37 CO2

Dolomite -0.83 -17.74 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.68 -2.83 O2

Initial solution 77. 30/8/2012 06:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.695e-004 3.695e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.182e-003

Total CO2 (mol/kg) = 4.182e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551907e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0242 0.8087

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.523e-008 8.791e-008 -7.021 -7.056 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.182e-003

HCO3- 3.596e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.265e-004 5.272e-004 -3.279 -3.278 0.001

CaHCO3+ 3.782e-005 3.503e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 2.915e-006 2.919e-006 -5.535 -5.535 0.001

CO3-2 2.848e-006 2.096e-006 -5.545 -5.679 -0.133

MgCO3 6.538e-007 6.546e-007 -6.185 -6.184 0.001

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaCO3- 2.645e-010 2.445e-010 -9.578 -9.612 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.431e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.782e-005 3.503e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 2.915e-006 2.919e-006 -5.535 -5.535 0.001

CaOH+ 2.684e-009 2.480e-009 -8.571 -8.605 -0.034

CaHSO4+ 4.606e-012 4.257e-012 -11.337 -11.371 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.078e-026

H2 3.039e-026 3.043e-026 -25.517 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.684e-013 1.687e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 6.538e-007 6.546e-007 -6.185 -6.184 0.001

MgOH+ 1.142e-008 1.055e-008 -7.942 -7.977 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.645e-010 2.445e-010 -9.578 -9.612 -0.034

NaOH 9.658e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 3.695e-004

O2 1.847e-004 1.850e-004 -3.733 -3.733 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 4.062e-010 3.754e-010 -9.391 -9.425 -0.034

CaHSO4+ 4.606e-012 4.257e-012 -11.337 -11.371 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.37 CO2

Dolomite -0.91 -17.82 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.90 -3.73 -2.83 O2

Initial solution 78. 30/8/2012 07:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.832e-004 3.832e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.210

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.169e-003

Total CO2 (mol/kg) = 4.169e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551906e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0181 0.8084

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.745e-008 8.996e-008 -7.011 -7.046 -0.035

H+ 6.621e-008 6.166e-008 -7.179 -7.210 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.169e-003

HCO3- 3.596e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.145e-004 5.151e-004 -3.289 -3.288 0.001

CaHCO3+ 3.782e-005 3.503e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 2.982e-006 2.986e-006 -5.525 -5.525 0.001

CO3-2 2.914e-006 2.144e-006 -5.536 -5.669 -0.133

MgCO3 6.690e-007 6.698e-007 -6.175 -6.174 0.001

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaCO3- 2.707e-010 2.502e-010 -9.568 -9.602 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.431e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.782e-005 3.503e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 2.982e-006 2.986e-006 -5.525 -5.525 0.001

CaOH+ 2.746e-009 2.538e-009 -8.561 -8.595 -0.034

CaHSO4+ 4.501e-012 4.160e-012 -11.347 -11.381 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.804e-026

H2 2.902e-026 2.906e-026 -25.537 -25.537 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.724e-013 1.726e-013 -12.764 -12.763 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 6.690e-007 6.698e-007 -6.175 -6.174 0.001

MgOH+ 1.168e-008 1.080e-008 -7.932 -7.967 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.707e-010 2.502e-010 -9.568 -9.602 -0.034

NaOH 9.883e-013 9.896e-013 -12.005 -12.005 0.001

O(0) 3.832e-004

O2 1.916e-004 1.919e-004 -3.718 -3.717 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.970e-010 3.669e-010 -9.401 -9.435 -0.034

CaHSO4+ 4.501e-012 4.160e-012 -11.347 -11.381 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.40 -8.69 -8.29 CaCO3

Calcite -0.25 -8.69 -8.44 CaCO3

CO2(g) -1.91 -3.29 -1.37 CO2

Dolomite -0.89 -17.80 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.42 -25.54 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.72 -2.83 O2

Initial solution 79. 30/8/2012 07:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.982e-004 3.982e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.158e-003

Total CO2 (mol/kg) = 4.158e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0123 0.8081

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.972e-008 9.205e-008 -7.001 -7.036 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.158e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.027e-004 5.034e-004 -3.299 -3.298 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.051e-006 3.055e-006 -5.516 -5.515 0.001

CO3-2 2.982e-006 2.194e-006 -5.526 -5.659 -0.133

MgCO3 6.845e-007 6.854e-007 -6.165 -6.164 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.770e-010 2.560e-010 -9.558 -9.592 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.051e-006 3.055e-006 -5.516 -5.515 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.399e-012 4.065e-012 -11.357 -11.391 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.543e-026

H2 2.771e-026 2.775e-026 -25.557 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 6.845e-007 6.854e-007 -6.165 -6.164 0.001

MgOH+ 1.195e-008 1.105e-008 -7.922 -7.957 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.770e-010 2.560e-010 -9.558 -9.592 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.982e-004

O2 1.991e-004 1.994e-004 -3.701 -3.700 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.059e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.879e-010 3.585e-010 -9.411 -9.445 -0.034

CaHSO4+ 4.399e-012 4.065e-012 -11.357 -11.391 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.37 CO2

Dolomite -0.87 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.70 -2.83 O2

Initial solution 80. 30/8/2012 07:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.882e-004 3.882e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551901e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9995 0.8073

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.882e-004

O2 1.941e-004 1.944e-004 -3.712 -3.711 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 81. 30/8/2012 07:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.651e-004 3.651e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.135e-003

Total CO2 (mol/kg) = 4.135e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551897e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9829 0.8064

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.044e-007 9.639e-008 -6.981 -7.016 -0.035

H+ 6.179e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.135e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.800e-004 4.806e-004 -3.319 -3.318 0.001

CaHCO3+ 3.780e-005 3.501e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.194e-006 3.198e-006 -5.496 -5.495 0.001

CO3-2 3.122e-006 2.297e-006 -5.506 -5.639 -0.133

MgCO3 7.166e-007 7.175e-007 -6.145 -6.144 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.780e-005 3.501e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.194e-006 3.198e-006 -5.496 -5.495 0.001

CaOH+ 2.942e-009 2.719e-009 -8.531 -8.566 -0.034

CaHSO4+ 4.200e-012 3.882e-012 -11.377 -11.411 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.055e-026

H2 2.528e-026 2.531e-026 -25.597 -25.597 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.166e-007 7.175e-007 -6.145 -6.144 0.001

MgOH+ 1.252e-008 1.157e-008 -7.902 -7.937 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 3.651e-004

O2 1.826e-004 1.828e-004 -3.739 -3.738 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.705e-010 3.424e-010 -9.431 -9.465 -0.034

CaHSO4+ 4.200e-012 3.882e-012 -11.377 -11.411 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.37 CO2

Dolomite -0.83 -17.74 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.90 -3.74 -2.83 O2

Initial solution 82. 30/8/2012 08:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.939e-004 3.939e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551902e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0011 0.8074

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.939e-004

O2 1.969e-004 1.972e-004 -3.706 -3.705 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.71 -2.83 O2

Initial solution 83. 30/8/2012 08:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.864e-004 3.864e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.135e-003

Total CO2 (mol/kg) = 4.135e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551899e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9890 0.8067

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.044e-007 9.639e-008 -6.981 -7.016 -0.035

H+ 6.179e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.135e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.800e-004 4.806e-004 -3.319 -3.318 0.001

CaHCO3+ 3.780e-005 3.501e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.194e-006 3.198e-006 -5.496 -5.495 0.001

CO3-2 3.122e-006 2.297e-006 -5.506 -5.639 -0.133

MgCO3 7.166e-007 7.175e-007 -6.145 -6.144 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.780e-005 3.501e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.194e-006 3.198e-006 -5.496 -5.495 0.001

CaOH+ 2.942e-009 2.719e-009 -8.531 -8.566 -0.034

CaHSO4+ 4.200e-012 3.882e-012 -11.377 -11.411 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.055e-026

H2 2.528e-026 2.531e-026 -25.597 -25.597 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.166e-007 7.175e-007 -6.145 -6.144 0.001

MgOH+ 1.252e-008 1.157e-008 -7.902 -7.937 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 3.864e-004

O2 1.932e-004 1.934e-004 -3.714 -3.713 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.705e-010 3.424e-010 -9.431 -9.465 -0.034

CaHSO4+ 4.200e-012 3.882e-012 -11.377 -11.411 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.37 CO2

Dolomite -0.83 -17.74 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 84. 30/8/2012 08:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.726e-004 3.726e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.135e-003

Total CO2 (mol/kg) = 4.135e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551897e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9851 0.8065

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.044e-007 9.639e-008 -6.981 -7.016 -0.035

H+ 6.179e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.135e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.800e-004 4.806e-004 -3.319 -3.318 0.001

CaHCO3+ 3.780e-005 3.501e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.194e-006 3.198e-006 -5.496 -5.495 0.001

CO3-2 3.122e-006 2.297e-006 -5.506 -5.639 -0.133

MgCO3 7.166e-007 7.175e-007 -6.145 -6.144 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.780e-005 3.501e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.194e-006 3.198e-006 -5.496 -5.495 0.001

CaOH+ 2.942e-009 2.719e-009 -8.531 -8.566 -0.034

CaHSO4+ 4.200e-012 3.882e-012 -11.377 -11.411 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.055e-026

H2 2.528e-026 2.531e-026 -25.597 -25.597 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.506e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.166e-007 7.175e-007 -6.145 -6.144 0.001

MgOH+ 1.252e-008 1.157e-008 -7.902 -7.937 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 3.726e-004

O2 1.863e-004 1.865e-004 -3.730 -3.729 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.705e-010 3.424e-010 -9.431 -9.465 -0.034

CaHSO4+ 4.200e-012 3.882e-012 -11.377 -11.411 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.37 CO2

Dolomite -0.83 -17.74 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.90 -3.73 -2.83 O2

Initial solution 85. 30/8/2012 08:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.714e-004 3.714e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551900e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9947 0.8070

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.714e-004

O2 1.857e-004 1.859e-004 -3.731 -3.731 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.90 -3.73 -2.83 O2

Initial solution 86. 30/8/2012 09:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.145e-004 4.145e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0066 0.8077

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.145e-004

O2 2.073e-004 2.075e-004 -3.684 -3.683 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.68 -2.83 O2

Initial solution 87. 30/8/2012 09:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.151e-004 4.151e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0068 0.8077

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.151e-004

O2 2.076e-004 2.078e-004 -3.683 -3.682 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.68 -2.83 O2

Initial solution 88. 30/8/2012 09:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.026e-004 4.026e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551903e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0035 0.8076

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.026e-004

O2 2.013e-004 2.016e-004 -3.696 -3.696 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 89. 30/8/2012 09:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.832e-004 3.832e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551901e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9981 0.8072

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.832e-004

O2 1.916e-004 1.919e-004 -3.718 -3.717 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.72 -2.83 O2

Initial solution 90. 30/8/2012 10:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.620e-004 3.620e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551899e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9919 0.8069

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.620e-004

O2 1.810e-004 1.812e-004 -3.742 -3.742 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.91 -3.74 -2.83 O2

Initial solution 91. 30/8/2012 10:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.001e-004 4.001e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551903e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0028 0.8075

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.001e-004

O2 2.001e-004 2.003e-004 -3.699 -3.698 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 92. 30/8/2012 10:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.776e-004 3.776e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99894

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.146e-003

Total CO2 (mol/kg) = 4.146e-003

Temperature (deg C) = 17.500

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551900e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9965 0.8072

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.020e-007 9.419e-008 -6.991 -7.026 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.146e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 4.912e-004 4.919e-004 -3.309 -3.308 0.001

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CO3-2 3.051e-006 2.245e-006 -5.516 -5.649 -0.133

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.781e-005 3.502e-005 -4.422 -4.456 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.122e-006 3.126e-006 -5.506 -5.505 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.293e-026

H2 2.647e-026 2.650e-026 -25.577 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.392e-005 -4.822 -4.856 -0.034

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

MgCO3 7.003e-007 7.012e-007 -6.155 -6.154 0.001

MgOH+ 1.223e-008 1.131e-008 -7.912 -7.947 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

NaCO3- 2.834e-010 2.619e-010 -9.548 -9.582 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.776e-004

O2 1.888e-004 1.891e-004 -3.724 -3.723 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.171e-005 -4.010 -4.144 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.058e-006 5.065e-006 -5.296 -5.295 0.001

NaSO4- 3.421e-009 3.162e-009 -8.466 -8.500 -0.034

KSO4- 1.463e-009 1.352e-009 -8.835 -8.869 -0.034

HSO4- 3.791e-010 3.504e-010 -9.421 -9.455 -0.034

CaHSO4+ 4.298e-012 3.972e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.37 CO2

Dolomite -0.85 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 93. 30/8/2012 10:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.782e-004 3.782e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.145e-003

Total CO2 (mol/kg) = 4.145e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551900e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9880 0.8069

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.029e-007 9.497e-008 -6.988 -7.022 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.145e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.904e-004 4.910e-004 -3.309 -3.309 0.001

CaHCO3+ 3.788e-005 3.508e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.134e-006 3.138e-006 -5.504 -5.503 0.001

CO3-2 3.058e-006 2.250e-006 -5.515 -5.648 -0.133

MgCO3 7.030e-007 7.039e-007 -6.153 -6.152 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.856e-010 2.639e-010 -9.544 -9.579 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.788e-005 3.508e-005 -4.422 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.134e-006 3.138e-006 -5.504 -5.503 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.306e-012 3.979e-012 -11.366 -11.400 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.288e-026

H2 2.644e-026 2.647e-026 -25.578 -25.577 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 7.030e-007 7.039e-007 -6.153 -6.152 0.001

MgOH+ 1.235e-008 1.141e-008 -7.908 -7.943 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.856e-010 2.639e-010 -9.544 -9.579 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.782e-004

O2 1.891e-004 1.894e-004 -3.723 -3.723 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.798e-010 3.510e-010 -9.420 -9.455 -0.034

CaHSO4+ 4.306e-012 3.979e-012 -11.366 -11.400 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.76 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.89 -3.72 -2.83 O2

Initial solution 94. 30/8/2012 11:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.895e-004 3.895e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.157e-003

Total CO2 (mol/kg) = 4.157e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0012 0.8077

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.005e-007 9.281e-008 -6.998 -7.032 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.157e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.019e-004 5.025e-004 -3.299 -3.299 0.001

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CO3-2 2.989e-006 2.199e-006 -5.524 -5.658 -0.133

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.537e-026

H2 2.769e-026 2.772e-026 -25.558 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

MgOH+ 1.207e-008 1.115e-008 -7.918 -7.953 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.895e-004

O2 1.947e-004 1.950e-004 -3.711 -3.710 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.886e-010 3.592e-010 -9.410 -9.445 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

Initial solution 95. 30/8/2012 11:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.901e-004 3.901e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.156e-003

Total CO2 (mol/kg) = 4.156e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551903e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9926 0.8075

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.014e-007 9.357e-008 -6.994 -7.029 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.156e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.010e-004 5.016e-004 -3.300 -3.300 0.001

CaHCO3+ 3.796e-005 3.516e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.074e-006 3.078e-006 -5.512 -5.512 0.001

CO3-2 2.996e-006 2.204e-006 -5.523 -5.657 -0.133

MgCO3 6.898e-007 6.906e-007 -6.161 -6.161 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.813e-010 2.599e-010 -9.551 -9.585 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.796e-005 3.516e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.074e-006 3.078e-006 -5.512 -5.512 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.413e-012 4.079e-012 -11.355 -11.389 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.531e-026

H2 2.766e-026 2.769e-026 -25.558 -25.558 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 6.898e-007 6.906e-007 -6.161 -6.161 0.001

MgOH+ 1.218e-008 1.126e-008 -7.914 -7.949 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.466 -8.500 -0.034

NaCO3- 2.813e-010 2.599e-010 -9.551 -9.585 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.901e-004

O2 1.951e-004 1.953e-004 -3.710 -3.709 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.466 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.894e-010 3.598e-010 -9.410 -9.444 -0.034

CaHSO4+ 4.413e-012 4.079e-012 -11.355 -11.389 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.77 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.87 -3.71 -2.84 O2

Initial solution 96. 30/8/2012 11:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.032e-004 4.032e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.157e-003

Total CO2 (mol/kg) = 4.157e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0049 0.8079

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.005e-007 9.281e-008 -6.998 -7.032 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.157e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.019e-004 5.025e-004 -3.299 -3.299 0.001

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CO3-2 2.989e-006 2.199e-006 -5.524 -5.658 -0.133

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.537e-026

H2 2.769e-026 2.772e-026 -25.558 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

MgOH+ 1.207e-008 1.115e-008 -7.918 -7.953 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.032e-004

O2 2.016e-004 2.019e-004 -3.695 -3.695 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.886e-010 3.592e-010 -9.410 -9.445 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.69 -2.83 O2

Initial solution 97. 30/8/2012 11:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.976e-004 3.976e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.156e-003

Total CO2 (mol/kg) = 4.156e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9947 0.8076

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.014e-007 9.357e-008 -6.994 -7.029 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.156e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.010e-004 5.016e-004 -3.300 -3.300 0.001

CaHCO3+ 3.796e-005 3.516e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.074e-006 3.078e-006 -5.512 -5.512 0.001

CO3-2 2.996e-006 2.204e-006 -5.523 -5.657 -0.133

MgCO3 6.898e-007 6.906e-007 -6.161 -6.161 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.813e-010 2.599e-010 -9.551 -9.585 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.796e-005 3.516e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.074e-006 3.078e-006 -5.512 -5.512 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.413e-012 4.079e-012 -11.355 -11.389 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.531e-026

H2 2.766e-026 2.769e-026 -25.558 -25.558 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 6.898e-007 6.906e-007 -6.161 -6.161 0.001

MgOH+ 1.218e-008 1.126e-008 -7.914 -7.949 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.466 -8.500 -0.034

NaCO3- 2.813e-010 2.599e-010 -9.551 -9.585 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.976e-004

O2 1.988e-004 1.991e-004 -3.702 -3.701 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.466 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.894e-010 3.598e-010 -9.410 -9.444 -0.034

CaHSO4+ 4.413e-012 4.079e-012 -11.355 -11.389 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.77 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.87 -3.70 -2.84 O2

Initial solution 98. 30/8/2012 12:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.820e-004 3.820e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.156e-003

Total CO2 (mol/kg) = 4.156e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551903e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9904 0.8074

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.014e-007 9.357e-008 -6.994 -7.029 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.156e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.010e-004 5.016e-004 -3.300 -3.300 0.001

CaHCO3+ 3.796e-005 3.516e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.074e-006 3.078e-006 -5.512 -5.512 0.001

CO3-2 2.996e-006 2.204e-006 -5.523 -5.657 -0.133

MgCO3 6.898e-007 6.906e-007 -6.161 -6.161 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.813e-010 2.599e-010 -9.551 -9.585 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.796e-005 3.516e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.074e-006 3.078e-006 -5.512 -5.512 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.413e-012 4.079e-012 -11.355 -11.389 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.531e-026

H2 2.766e-026 2.769e-026 -25.558 -25.558 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 6.898e-007 6.906e-007 -6.161 -6.161 0.001

MgOH+ 1.218e-008 1.126e-008 -7.914 -7.949 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.466 -8.500 -0.034

NaCO3- 2.813e-010 2.599e-010 -9.551 -9.585 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.820e-004

O2 1.910e-004 1.912e-004 -3.719 -3.718 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.466 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.894e-010 3.598e-010 -9.410 -9.444 -0.034

CaHSO4+ 4.413e-012 4.079e-012 -11.355 -11.389 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.77 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.88 -3.72 -2.84 O2

Initial solution 99. 30/8/2012 12:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.058e-004 4.058e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.156e-003

Total CO2 (mol/kg) = 4.156e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9969 0.8077

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.014e-007 9.357e-008 -6.994 -7.029 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.156e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.010e-004 5.016e-004 -3.300 -3.300 0.001

CaHCO3+ 3.796e-005 3.516e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.074e-006 3.078e-006 -5.512 -5.512 0.001

CO3-2 2.996e-006 2.204e-006 -5.523 -5.657 -0.133

MgCO3 6.898e-007 6.906e-007 -6.161 -6.161 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.813e-010 2.599e-010 -9.551 -9.585 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.796e-005 3.516e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.074e-006 3.078e-006 -5.512 -5.512 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.413e-012 4.079e-012 -11.355 -11.389 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.531e-026

H2 2.766e-026 2.769e-026 -25.558 -25.558 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 6.898e-007 6.906e-007 -6.161 -6.161 0.001

MgOH+ 1.218e-008 1.126e-008 -7.914 -7.949 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.466 -8.500 -0.034

NaCO3- 2.813e-010 2.599e-010 -9.551 -9.585 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.058e-004

O2 2.029e-004 2.031e-004 -3.693 -3.692 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.466 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.894e-010 3.598e-010 -9.410 -9.444 -0.034

CaHSO4+ 4.413e-012 4.079e-012 -11.355 -11.389 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.77 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.86 -3.69 -2.84 O2

Initial solution 100. 30/8/2012 12:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.114e-004 4.114e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.608e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.143e-003

Total CO2 (mol/kg) = 4.143e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.02

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551902e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9897 0.8076

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.022e-007 9.434e-008 -6.991 -7.025 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.143e-003

HCO3- 3.585e-003 3.320e-003 -2.446 -2.479 -0.033

CO2 4.987e-004 4.994e-004 -3.302 -3.302 0.001

CaHCO3+ 3.783e-005 3.504e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

CaCO3 3.069e-006 3.073e-006 -5.513 -5.512 0.001

CO3-2 2.994e-006 2.204e-006 -5.524 -5.657 -0.133

MgCO3 6.907e-007 6.916e-007 -6.161 -6.160 0.001

NaHCO3 1.722e-008 1.725e-008 -7.764 -7.763 0.001

NaCO3- 2.826e-010 2.612e-010 -9.549 -9.583 -0.034

Ca 1.332e-003

Ca+2 1.279e-003 9.404e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.783e-005 3.504e-005 -4.422 -4.455 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.069e-006 3.073e-006 -5.513 -5.512 0.001

CaOH+ 2.802e-009 2.590e-009 -8.552 -8.587 -0.034

CaHSO4+ 4.412e-012 4.078e-012 -11.355 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 5.526e-026

H2 2.763e-026 2.766e-026 -25.559 -25.558 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.471e-009 1.359e-009 -8.832 -8.867 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

MgSO4 5.099e-006 5.106e-006 -5.292 -5.292 0.001

MgCO3 6.907e-007 6.916e-007 -6.161 -6.160 0.001

MgOH+ 1.230e-008 1.137e-008 -7.910 -7.944 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.722e-008 1.725e-008 -7.764 -7.763 0.001

NaSO4- 3.427e-009 3.167e-009 -8.465 -8.499 -0.034

NaCO3- 2.826e-010 2.612e-010 -9.549 -9.583 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.114e-004

O2 2.057e-004 2.060e-004 -3.687 -3.686 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.099e-006 5.106e-006 -5.292 -5.292 0.001

NaSO4- 3.427e-009 3.167e-009 -8.465 -8.499 -0.034

KSO4- 1.471e-009 1.359e-009 -8.832 -8.867 -0.034

HSO4- 3.902e-010 3.607e-010 -9.409 -9.443 -0.034

CaHSO4+ 4.412e-012 4.078e-012 -11.355 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.85 -3.69 -2.84 O2

Initial solution 101. 30/8/2012 12:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.208e-004 4.208e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 297

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.143e-003

Total CO2 (mol/kg) = 4.143e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9821 0.8072

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.046e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.143e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.887e-004 4.893e-004 -3.311 -3.310 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CO3-2 3.073e-006 2.261e-006 -5.512 -5.646 -0.133

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.427e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

MgOH+ 1.258e-008 1.163e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.208e-004

O2 2.104e-004 2.107e-004 -3.677 -3.676 0.001

S(6) 1.154e-004

SO4-2 9.771e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

HSO4- 3.812e-010 3.523e-010 -9.419 -9.453 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.83 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.84 -3.68 -2.84 O2

Initial solution 102. 30/8/2012 13:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.651e-003 3.651e-003

Ca 1.332e-003 1.332e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.201e-004 4.201e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.608e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.132e-003

Total CO2 (mol/kg) = 4.132e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.250e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.02

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551901e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9820 0.8071

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.046e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.322e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.132e-003

HCO3- 3.584e-003 3.320e-003 -2.446 -2.479 -0.033

CO2 4.873e-004 4.880e-004 -3.312 -3.312 0.001

CaHCO3+ 3.783e-005 3.504e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

CaCO3 3.140e-006 3.144e-006 -5.503 -5.502 0.001

CO3-2 3.064e-006 2.255e-006 -5.514 -5.647 -0.133

MgCO3 7.067e-007 7.077e-007 -6.151 -6.150 0.001

NaHCO3 1.722e-008 1.724e-008 -7.764 -7.763 0.001

NaCO3- 2.892e-010 2.673e-010 -9.539 -9.573 -0.034

Ca 1.332e-003

Ca+2 1.278e-003 9.404e-004 -2.893 -3.027 -0.133

CaHCO3+ 3.783e-005 3.504e-005 -4.422 -4.455 -0.033

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

CaCO3 3.140e-006 3.144e-006 -5.503 -5.502 0.001

CaOH+ 2.867e-009 2.650e-009 -8.543 -8.577 -0.034

CaHSO4+ 4.311e-012 3.985e-012 -11.365 -11.400 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.471e-009 1.359e-009 -8.832 -8.867 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.674e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.504e-005 1.390e-005 -4.823 -4.857 -0.034

MgSO4 5.099e-006 5.106e-006 -5.292 -5.292 0.001

MgCO3 7.067e-007 7.077e-007 -6.151 -6.150 0.001

MgOH+ 1.259e-008 1.163e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.237e-006 -5.001 -5.034 -0.034

NaHCO3 1.722e-008 1.724e-008 -7.764 -7.763 0.001

NaSO4- 3.427e-009 3.167e-009 -8.465 -8.499 -0.034

NaCO3- 2.892e-010 2.673e-010 -9.539 -9.573 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.201e-004

O2 2.101e-004 2.103e-004 -3.678 -3.677 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.170e-005 -4.010 -4.145 -0.135

CaSO4 1.254e-005 1.256e-005 -4.902 -4.901 0.001

MgSO4 5.099e-006 5.106e-006 -5.292 -5.292 0.001

NaSO4- 3.427e-009 3.167e-009 -8.465 -8.499 -0.034

KSO4- 1.471e-009 1.359e-009 -8.832 -8.867 -0.034

HSO4- 3.813e-010 3.525e-010 -9.419 -9.453 -0.034

CaHSO4+ 4.311e-012 3.985e-012 -11.365 -11.400 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.76 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.84 -3.68 -2.84 O2

Initial solution 103. 30/8/2012 13:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.932e-004 3.932e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.144e-003

Total CO2 (mol/kg) = 4.144e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551901e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9835 0.8070

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.037e-007 9.575e-008 -6.984 -7.019 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.144e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.895e-004 4.902e-004 -3.310 -3.310 0.001

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CO3-2 3.066e-006 2.256e-006 -5.513 -5.647 -0.133

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.282e-026

H2 2.641e-026 2.645e-026 -25.578 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

MgOH+ 1.247e-008 1.152e-008 -7.904 -7.939 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.932e-004

O2 1.966e-004 1.969e-004 -3.706 -3.706 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.805e-010 3.516e-010 -9.420 -9.454 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.87 -3.71 -2.84 O2

Initial solution 104. 30/8/2012 13:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.239e-004 4.239e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 297

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.143e-003

Total CO2 (mol/kg) = 4.143e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551904e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9829 0.8072

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.046e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.143e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.887e-004 4.893e-004 -3.311 -3.310 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CO3-2 3.073e-006 2.261e-006 -5.512 -5.646 -0.133

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.427e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

MgOH+ 1.258e-008 1.163e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.239e-004

O2 2.119e-004 2.122e-004 -3.674 -3.673 0.001

S(6) 1.154e-004

SO4-2 9.771e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

HSO4- 3.812e-010 3.523e-010 -9.419 -9.453 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.83 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.84 -3.67 -2.84 O2

Initial solution 105. 30/8/2012 13:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.951e-004 3.951e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 297

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.132e-003

Total CO2 (mol/kg) = 4.132e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551899e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9653 0.8062

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.070e-007 9.878e-008 -6.971 -7.005 -0.035

H+ 6.179e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.132e-003

HCO3- 3.594e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.775e-004 4.781e-004 -3.321 -3.320 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.230e-006 3.234e-006 -5.491 -5.490 0.001

CO3-2 3.144e-006 2.313e-006 -5.502 -5.636 -0.133

MgCO3 7.249e-007 7.258e-007 -6.140 -6.139 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.967e-010 2.742e-010 -9.528 -9.562 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.426e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.230e-006 3.234e-006 -5.491 -5.490 0.001

CaOH+ 2.941e-009 2.718e-009 -8.531 -8.566 -0.034

CaHSO4+ 4.222e-012 3.902e-012 -11.375 -11.409 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.039e-026

H2 2.520e-026 2.523e-026 -25.599 -25.598 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

MgCO3 7.249e-007 7.258e-007 -6.140 -6.139 0.001

MgOH+ 1.288e-008 1.190e-008 -7.890 -7.924 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

NaCO3- 2.967e-010 2.742e-010 -9.528 -9.562 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 3.951e-004

O2 1.976e-004 1.978e-004 -3.704 -3.704 0.001

S(6) 1.154e-004

SO4-2 9.771e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

HSO4- 3.725e-010 3.443e-010 -9.429 -9.463 -0.034

CaHSO4+ 4.222e-012 3.902e-012 -11.375 -11.409 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.38 CO2

Dolomite -0.81 -17.73 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.87 -3.70 -2.84 O2

Initial solution 106. 30/8/2012 14:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.039e-004 4.039e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 297

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.143e-003

Total CO2 (mol/kg) = 4.143e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551902e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9777 0.8069

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.046e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.143e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.887e-004 4.893e-004 -3.311 -3.310 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CO3-2 3.073e-006 2.261e-006 -5.512 -5.646 -0.133

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.427e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

MgOH+ 1.258e-008 1.163e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.039e-004

O2 2.019e-004 2.022e-004 -3.695 -3.694 0.001

S(6) 1.154e-004

SO4-2 9.771e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

HSO4- 3.812e-010 3.523e-010 -9.419 -9.453 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.83 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.86 -3.69 -2.84 O2

Initial solution 107. 30/8/2012 14:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.982e-004 3.982e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.240

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 297

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.132e-003

Total CO2 (mol/kg) = 4.132e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551900e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9662 0.8062

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.070e-007 9.878e-008 -6.971 -7.005 -0.035

H+ 6.179e-008 5.754e-008 -7.209 -7.240 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.132e-003

HCO3- 3.594e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.775e-004 4.781e-004 -3.321 -3.320 0.001

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.230e-006 3.234e-006 -5.491 -5.490 0.001

CO3-2 3.144e-006 2.313e-006 -5.502 -5.636 -0.133

MgCO3 7.249e-007 7.258e-007 -6.140 -6.139 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.967e-010 2.742e-010 -9.528 -9.562 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.426e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.802e-005 3.521e-005 -4.420 -4.453 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.230e-006 3.234e-006 -5.491 -5.490 0.001

CaOH+ 2.941e-009 2.718e-009 -8.531 -8.566 -0.034

CaHSO4+ 4.222e-012 3.902e-012 -11.375 -11.409 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.039e-026

H2 2.520e-026 2.523e-026 -25.599 -25.598 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

KOH 1.847e-013 1.849e-013 -12.734 -12.733 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

MgCO3 7.249e-007 7.258e-007 -6.140 -6.139 0.001

MgOH+ 1.288e-008 1.190e-008 -7.890 -7.924 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

NaCO3- 2.967e-010 2.742e-010 -9.528 -9.562 -0.034

NaOH 1.059e-012 1.060e-012 -11.975 -11.975 0.001

O(0) 3.982e-004

O2 1.991e-004 1.994e-004 -3.701 -3.700 0.001

S(6) 1.154e-004

SO4-2 9.771e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

HSO4- 3.725e-010 3.443e-010 -9.429 -9.463 -0.034

CaHSO4+ 4.222e-012 3.902e-012 -11.375 -11.409 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.37 -8.66 -8.29 CaCO3

Calcite -0.22 -8.66 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.38 CO2

Dolomite -0.81 -17.73 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.48 -25.60 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.86 -3.70 -2.84 O2

Initial solution 108. 30/8/2012 14:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.801e-004 3.801e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 297

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.143e-003

Total CO2 (mol/kg) = 4.143e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551900e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9711 0.8065

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.046e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.143e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.887e-004 4.893e-004 -3.311 -3.310 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CO3-2 3.073e-006 2.261e-006 -5.512 -5.646 -0.133

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.427e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

MgOH+ 1.258e-008 1.163e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.801e-004

O2 1.901e-004 1.903e-004 -3.721 -3.721 0.001

S(6) 1.154e-004

SO4-2 9.771e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

HSO4- 3.812e-010 3.523e-010 -9.419 -9.453 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.83 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.88 -3.72 -2.84 O2

Initial solution 109. 30/8/2012 15:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.045e-004 4.045e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 298

Density (g/cm3) = 0.99887

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.142e-003

Total CO2 (mol/kg) = 4.142e-003

Temperature (deg C) = 17.900

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551902e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9692 0.8067

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.054e-007 9.732e-008 -6.977 -7.012 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.142e-003

HCO3- 3.594e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.879e-004 4.885e-004 -3.312 -3.311 0.001

CaHCO3+ 3.810e-005 3.529e-005 -4.419 -4.452 -0.033

MgHCO3+ 1.508e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.168e-006 3.173e-006 -5.499 -5.499 0.001

CO3-2 3.080e-006 2.266e-006 -5.511 -5.645 -0.133

MgCO3 7.112e-007 7.121e-007 -6.148 -6.147 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.922e-010 2.701e-010 -9.534 -9.569 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.426e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.810e-005 3.529e-005 -4.419 -4.452 -0.033

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

CaCO3 3.168e-006 3.173e-006 -5.499 -5.499 0.001

CaOH+ 2.874e-009 2.656e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.328e-012 3.999e-012 -11.364 -11.398 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.271e-026

H2 2.636e-026 2.639e-026 -25.579 -25.579 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.473e-009 1.361e-009 -8.832 -8.866 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.508e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.107e-006 5.114e-006 -5.292 -5.291 0.001

MgCO3 7.112e-007 7.121e-007 -6.148 -6.147 0.001

MgOH+ 1.270e-008 1.174e-008 -7.896 -7.930 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.427e-009 3.167e-009 -8.465 -8.499 -0.034

NaCO3- 2.922e-010 2.701e-010 -9.534 -9.569 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 4.045e-004

O2 2.023e-004 2.025e-004 -3.694 -3.694 0.001

S(6) 1.154e-004

SO4-2 9.769e-005 7.164e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

MgSO4 5.107e-006 5.114e-006 -5.292 -5.291 0.001

NaSO4- 3.427e-009 3.167e-009 -8.465 -8.499 -0.034

KSO4- 1.473e-009 1.361e-009 -8.832 -8.866 -0.034

HSO4- 3.819e-010 3.529e-010 -9.418 -9.452 -0.034

CaHSO4+ 4.328e-012 3.999e-012 -11.364 -11.398 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.83 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.86 -3.69 -2.84 O2

Initial solution 110. 30/8/2012 15:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.620e-003 3.620e-003

Ca 1.321e-003 1.321e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.645e-004 3.645e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 294

Density (g/cm3) = 0.99888

Activity of water = 1.000

Ionic strength = 5.572e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.097e-003

Total CO2 (mol/kg) = 4.097e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.165e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.92

Iterations = 7

Total H = 1.110160e+002

Total O = 5.551885e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9666 0.8063

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.045e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.321e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.097e-003

HCO3- 3.554e-003 3.293e-003 -2.449 -2.482 -0.033

CO2 4.834e-004 4.840e-004 -3.316 -3.315 0.001

CaHCO3+ 3.723e-005 3.449e-005 -4.429 -4.462 -0.033

MgHCO3+ 1.493e-005 1.380e-005 -4.826 -4.860 -0.034

CaCO3 3.092e-006 3.096e-006 -5.510 -5.509 0.001

CO3-2 3.036e-006 2.236e-006 -5.518 -5.650 -0.133

MgCO3 7.017e-007 7.026e-007 -6.154 -6.153 0.001

NaHCO3 1.708e-008 1.711e-008 -7.767 -7.767 0.001

NaCO3- 2.868e-010 2.652e-010 -9.542 -9.576 -0.034

Ca 1.321e-003

Ca+2 1.268e-003 9.335e-004 -2.897 -3.030 -0.133

CaHCO3+ 3.723e-005 3.449e-005 -4.429 -4.462 -0.033

CaSO4 1.247e-005 1.248e-005 -4.904 -4.904 0.001

CaCO3 3.092e-006 3.096e-006 -5.510 -5.509 0.001

CaOH+ 2.846e-009 2.631e-009 -8.546 -8.580 -0.034

CaHSO4+ 4.285e-012 3.961e-012 -11.368 -11.402 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.290e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.070e-006 -5.478 -5.513 -0.035

KSO4- 1.473e-009 1.362e-009 -8.832 -8.866 -0.034

KOH 1.805e-013 1.808e-013 -12.743 -12.743 0.001

Mg 5.184e-004

Mg+2 4.977e-004 3.678e-004 -3.303 -3.434 -0.131

MgHCO3+ 1.493e-005 1.380e-005 -4.826 -4.860 -0.034

MgSO4 5.112e-006 5.119e-006 -5.291 -5.291 0.001

MgCO3 7.017e-007 7.026e-007 -6.154 -6.153 0.001

MgOH+ 1.260e-008 1.165e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.239e-006 -5.001 -5.034 -0.034

NaHCO3 1.708e-008 1.711e-008 -7.767 -7.767 0.001

NaSO4- 3.432e-009 3.173e-009 -8.464 -8.499 -0.034

NaCO3- 2.868e-010 2.652e-010 -9.542 -9.576 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.984 0.001

O(0) 3.645e-004

O2 1.822e-004 1.825e-004 -3.739 -3.739 0.001

S(6) 1.154e-004

SO4-2 9.779e-005 7.180e-005 -4.010 -4.144 -0.134

CaSO4 1.247e-005 1.248e-005 -4.904 -4.904 0.001

MgSO4 5.112e-006 5.119e-006 -5.291 -5.291 0.001

NaSO4- 3.432e-009 3.173e-009 -8.464 -8.499 -0.034

KSO4- 1.473e-009 1.362e-009 -8.832 -8.866 -0.034

HSO4- 3.818e-010 3.530e-010 -9.418 -9.452 -0.034

CaHSO4+ 4.285e-012 3.961e-012 -11.368 -11.402 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.94 -3.32 -1.38 CO2

Dolomite -0.85 -17.77 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.90 -3.74 -2.84 O2

Initial solution 111. 30/8/2012 15:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.839e-004 3.839e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 297

Density (g/cm3) = 0.99889

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.143e-003

Total CO2 (mol/kg) = 4.143e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551900e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9722 0.8066

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.046e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.143e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.887e-004 4.893e-004 -3.311 -3.310 0.001

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CO3-2 3.073e-006 2.261e-006 -5.512 -5.646 -0.133

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.427e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.803e-005 3.522e-005 -4.420 -4.453 -0.033

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

CaCO3 3.157e-006 3.161e-006 -5.501 -5.500 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

MgCO3 7.085e-007 7.094e-007 -6.150 -6.149 0.001

MgOH+ 1.258e-008 1.163e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

NaCO3- 2.900e-010 2.680e-010 -9.538 -9.572 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.839e-004

O2 1.919e-004 1.922e-004 -3.717 -3.716 0.001

S(6) 1.154e-004

SO4-2 9.771e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.258e-005 -4.901 -4.900 0.001

MgSO4 5.095e-006 5.101e-006 -5.293 -5.292 0.001

NaSO4- 3.425e-009 3.165e-009 -8.465 -8.500 -0.034

KSO4- 1.470e-009 1.359e-009 -8.833 -8.867 -0.034

HSO4- 3.812e-010 3.523e-010 -9.419 -9.453 -0.034

CaHSO4+ 4.320e-012 3.993e-012 -11.364 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.83 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.88 -3.72 -2.84 O2

Initial solution 112. 30/8/2012 15:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.631e-003 3.631e-003

Ca 1.325e-003 1.325e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.939e-004 3.939e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99888

Activity of water = 1.000

Ionic strength = 5.584e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.108e-003

Total CO2 (mol/kg) = 4.108e-003

Temperature (deg C) = 17.800

Electrical balance (eq) = -2.195e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.95

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551891e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9750 0.8067

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.046e-007 9.653e-008 -6.981 -7.015 -0.035

H+ 6.322e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.108e-003

HCO3- 3.564e-003 3.302e-003 -2.448 -2.481 -0.033

CO2 4.847e-004 4.853e-004 -3.315 -3.314 0.001

CaHCO3+ 3.743e-005 3.468e-005 -4.427 -4.460 -0.033

MgHCO3+ 1.496e-005 1.383e-005 -4.825 -4.859 -0.034

CaCO3 3.108e-006 3.112e-006 -5.508 -5.507 0.001

CO3-2 3.045e-006 2.242e-006 -5.516 -5.649 -0.133

MgCO3 7.034e-007 7.043e-007 -6.153 -6.152 0.001

NaHCO3 1.713e-008 1.715e-008 -7.766 -7.766 0.001

NaCO3- 2.876e-010 2.659e-010 -9.541 -9.575 -0.034

Ca 1.325e-003

Ca+2 1.271e-003 9.358e-004 -2.896 -3.029 -0.133

CaHCO3+ 3.743e-005 3.468e-005 -4.427 -4.460 -0.033

CaSO4 1.249e-005 1.251e-005 -4.903 -4.903 0.001

CaCO3 3.108e-006 3.112e-006 -5.508 -5.507 0.001

CaOH+ 2.853e-009 2.637e-009 -8.545 -8.579 -0.034

CaHSO4+ 4.294e-012 3.969e-012 -11.367 -11.401 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.289e-005 -4.242 -4.277 -0.035

H(0) 5.277e-026

H2 2.638e-026 2.642e-026 -25.579 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.070e-006 -5.478 -5.513 -0.035

KSO4- 1.472e-009 1.361e-009 -8.832 -8.866 -0.034

KOH 1.805e-013 1.807e-013 -12.743 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.676e-004 -3.303 -3.435 -0.131

MgHCO3+ 1.496e-005 1.383e-005 -4.825 -4.859 -0.034

MgSO4 5.108e-006 5.115e-006 -5.292 -5.291 0.001

MgCO3 7.034e-007 7.043e-007 -6.153 -6.152 0.001

MgOH+ 1.259e-008 1.164e-008 -7.900 -7.934 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.238e-006 -5.001 -5.034 -0.034

NaHCO3 1.713e-008 1.715e-008 -7.766 -7.766 0.001

NaSO4- 3.430e-009 3.171e-009 -8.465 -8.499 -0.034

NaCO3- 2.876e-010 2.659e-010 -9.541 -9.575 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.984 0.001

O(0) 3.939e-004

O2 1.969e-004 1.972e-004 -3.706 -3.705 0.001

S(6) 1.154e-004

SO4-2 9.777e-005 7.177e-005 -4.010 -4.144 -0.134

CaSO4 1.249e-005 1.251e-005 -4.903 -4.903 0.001

MgSO4 5.108e-006 5.115e-006 -5.292 -5.291 0.001

NaSO4- 3.430e-009 3.171e-009 -8.465 -8.499 -0.034

KSO4- 1.472e-009 1.361e-009 -8.832 -8.866 -0.034

HSO4- 3.817e-010 3.528e-010 -9.418 -9.452 -0.034

CaHSO4+ 4.294e-012 3.969e-012 -11.367 -11.401 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.94 -3.31 -1.38 CO2

Dolomite -0.84 -17.76 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.87 -3.71 -2.84 O2

Initial solution 113. 30/8/2012 16:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.957e-004 3.957e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.144e-003

Total CO2 (mol/kg) = 4.144e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551902e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9842 0.8070

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.037e-007 9.575e-008 -6.984 -7.019 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.144e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.895e-004 4.902e-004 -3.310 -3.310 0.001

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CO3-2 3.066e-006 2.256e-006 -5.513 -5.647 -0.133

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.282e-026

H2 2.641e-026 2.645e-026 -25.578 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

MgOH+ 1.247e-008 1.152e-008 -7.904 -7.939 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.957e-004

O2 1.979e-004 1.981e-004 -3.704 -3.703 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.805e-010 3.516e-010 -9.420 -9.454 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.87 -3.70 -2.84 O2

Initial solution 114. 30/8/2012 16:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.670e-004 3.670e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.144e-003

Total CO2 (mol/kg) = 4.144e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551899e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9760 0.8065

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.037e-007 9.575e-008 -6.984 -7.019 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.144e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.895e-004 4.902e-004 -3.310 -3.310 0.001

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CO3-2 3.066e-006 2.256e-006 -5.513 -5.647 -0.133

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.282e-026

H2 2.641e-026 2.645e-026 -25.578 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

MgOH+ 1.247e-008 1.152e-008 -7.904 -7.939 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.670e-004

O2 1.835e-004 1.837e-004 -3.736 -3.736 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.805e-010 3.516e-010 -9.420 -9.454 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.90 -3.74 -2.84 O2

Initial solution 115. 30/8/2012 16:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.945e-004 3.945e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.230

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99890

Activity of water = 1.000

Ionic strength = 5.620e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.144e-003

Total CO2 (mol/kg) = 4.144e-003

Temperature (deg C) = 17.700

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551902e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 13.9839 0.8070

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.037e-007 9.575e-008 -6.984 -7.019 -0.035

H+ 6.323e-008 5.888e-008 -7.199 -7.230 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.144e-003

HCO3- 3.595e-003 3.329e-003 -2.444 -2.478 -0.033

CO2 4.895e-004 4.902e-004 -3.310 -3.310 0.001

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CO3-2 3.066e-006 2.256e-006 -5.513 -5.647 -0.133

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.428e-004 -2.892 -3.026 -0.134

CaHCO3+ 3.795e-005 3.515e-005 -4.421 -4.454 -0.033

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.145e-006 3.149e-006 -5.502 -5.502 0.001

CaOH+ 2.875e-009 2.657e-009 -8.541 -8.576 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.282e-026

H2 2.641e-026 2.645e-026 -25.578 -25.578 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

KOH 1.805e-013 1.807e-013 -12.744 -12.743 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

MgCO3 7.057e-007 7.067e-007 -6.151 -6.151 0.001

MgOH+ 1.247e-008 1.152e-008 -7.904 -7.939 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

NaCO3- 2.878e-010 2.660e-010 -9.541 -9.575 -0.034

NaOH 1.035e-012 1.036e-012 -11.985 -11.985 0.001

O(0) 3.945e-004

O2 1.972e-004 1.975e-004 -3.705 -3.704 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.168e-005 -4.010 -4.145 -0.135

CaSO4 1.256e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.083e-006 5.089e-006 -5.294 -5.293 0.001

NaSO4- 3.424e-009 3.164e-009 -8.465 -8.500 -0.034

KSO4- 1.468e-009 1.357e-009 -8.833 -8.868 -0.034

HSO4- 3.805e-010 3.516e-010 -9.420 -9.454 -0.034

CaHSO4+ 4.313e-012 3.986e-012 -11.365 -11.399 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.38 -8.67 -8.29 CaCO3

Calcite -0.23 -8.67 -8.44 CaCO3

CO2(g) -1.93 -3.31 -1.38 CO2

Dolomite -0.84 -17.75 -16.92 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.46 -25.58 -3.12 H2

H2O(g) -1.70 -0.00 1.70 H2O

Halite -10.88 -9.31 1.57 NaCl

O2(g) -0.87 -3.70 -2.84 O2

Initial solution 116. 30/8/2012 16:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.976e-004 3.976e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.168e-003

Total CO2 (mol/kg) = 4.168e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551908e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0034 0.8078

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.005e-007 9.281e-008 -6.998 -7.032 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.168e-003

HCO3- 3.605e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.032e-004 5.039e-004 -3.298 -3.298 0.001

CaHCO3+ 3.809e-005 3.527e-005 -4.419 -4.453 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 3.078e-006 3.082e-006 -5.512 -5.511 0.001

CO3-2 2.998e-006 2.205e-006 -5.523 -5.657 -0.133

MgCO3 6.887e-007 6.896e-007 -6.162 -6.161 0.001

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaCO3- 2.799e-010 2.586e-010 -9.553 -9.587 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.452e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.809e-005 3.527e-005 -4.419 -4.453 -0.033

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

CaCO3 3.078e-006 3.082e-006 -5.512 -5.511 0.001

CaOH+ 2.817e-009 2.603e-009 -8.550 -8.585 -0.034

CaHSO4+ 4.415e-012 4.080e-012 -11.355 -11.389 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.537e-026

H2 2.769e-026 2.772e-026 -25.558 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.465e-009 1.354e-009 -8.834 -8.869 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.975e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.066e-006 5.073e-006 -5.295 -5.295 0.001

MgCO3 6.887e-007 6.896e-007 -6.162 -6.161 0.001

MgOH+ 1.206e-008 1.115e-008 -7.918 -7.953 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.762 -7.761 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.799e-010 2.586e-010 -9.553 -9.587 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.976e-004

O2 1.988e-004 1.991e-004 -3.702 -3.701 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

MgSO4 5.066e-006 5.073e-006 -5.295 -5.295 0.001

NaSO4- 3.421e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.465e-009 1.354e-009 -8.834 -8.869 -0.034

HSO4- 3.885e-010 3.590e-010 -9.411 -9.445 -0.034

CaHSO4+ 4.415e-012 4.080e-012 -11.355 -11.389 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.77 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.87 -3.70 -2.83 O2

Initial solution 117. 30/8/2012 17:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.014e-004 4.014e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.181e-003

Total CO2 (mol/kg) = 4.181e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551910e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0244 0.8090

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.601e-008 8.863e-008 -7.018 -7.052 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.181e-003

HCO3- 3.596e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.256e-004 5.263e-004 -3.279 -3.279 0.001

CaHCO3+ 3.790e-005 3.510e-005 -4.421 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 2.926e-006 2.929e-006 -5.534 -5.533 0.001

CO3-2 2.855e-006 2.101e-006 -5.544 -5.678 -0.133

MgCO3 6.563e-007 6.572e-007 -6.183 -6.182 0.001

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaCO3- 2.666e-010 2.464e-010 -9.574 -9.608 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.430e-004 -2.892 -3.025 -0.133

CaHCO3+ 3.790e-005 3.510e-005 -4.421 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 2.926e-006 2.929e-006 -5.534 -5.533 0.001

CaOH+ 2.684e-009 2.480e-009 -8.571 -8.606 -0.034

CaHSO4+ 4.614e-012 4.264e-012 -11.336 -11.370 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.071e-026

H2 3.036e-026 3.040e-026 -25.518 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.465e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.563e-007 6.572e-007 -6.183 -6.182 0.001

MgOH+ 1.153e-008 1.065e-008 -7.938 -7.973 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.730e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.666e-010 2.464e-010 -9.574 -9.608 -0.034

NaOH 9.658e-013 9.670e-013 -12.015 -12.015 0.001

O(0) 4.014e-004

O2 2.007e-004 2.009e-004 -3.697 -3.697 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.465e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 4.070e-010 3.761e-010 -9.390 -9.425 -0.034

CaHSO4+ 4.614e-012 4.264e-012 -11.336 -11.370 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.38 CO2

Dolomite -0.90 -17.82 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 118. 30/8/2012 17:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.083e-004 4.083e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.157e-003

Total CO2 (mol/kg) = 4.157e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0063 0.8080

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.005e-007 9.281e-008 -6.998 -7.032 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.157e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.019e-004 5.025e-004 -3.299 -3.299 0.001

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CO3-2 2.989e-006 2.199e-006 -5.524 -5.658 -0.133

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.537e-026

H2 2.769e-026 2.772e-026 -25.558 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

MgOH+ 1.207e-008 1.115e-008 -7.918 -7.953 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 4.083e-004

O2 2.041e-004 2.044e-004 -3.690 -3.690 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.886e-010 3.592e-010 -9.410 -9.445 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.85 -3.69 -2.83 O2

Initial solution 119. 30/8/2012 17:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.662e-003 3.662e-003

Ca 1.336e-003 1.336e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.995e-004 3.995e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.220

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 295

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.157e-003

Total CO2 (mol/kg) = 4.157e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.280e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.05

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551905e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0039 0.8079

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.005e-007 9.281e-008 -6.998 -7.032 -0.035

H+ 6.470e-008 6.026e-008 -7.189 -7.220 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.157e-003

HCO3- 3.595e-003 3.330e-003 -2.444 -2.478 -0.033

CO2 5.019e-004 5.025e-004 -3.299 -3.299 0.001

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CO3-2 2.989e-006 2.199e-006 -5.524 -5.658 -0.133

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

Ca 1.336e-003

Ca+2 1.282e-003 9.429e-004 -2.892 -3.026 -0.133

CaHCO3+ 3.789e-005 3.509e-005 -4.422 -4.455 -0.033

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

CaCO3 3.063e-006 3.067e-006 -5.514 -5.513 0.001

CaOH+ 2.810e-009 2.597e-009 -8.551 -8.586 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 5.537e-026

H2 2.769e-026 2.772e-026 -25.558 -25.557 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

KOH 1.764e-013 1.766e-013 -12.754 -12.753 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.673e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.507e-005 1.393e-005 -4.822 -4.856 -0.034

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

MgCO3 6.871e-007 6.880e-007 -6.163 -6.162 0.001

MgOH+ 1.207e-008 1.115e-008 -7.918 -7.953 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.236e-006 -5.001 -5.035 -0.034

NaHCO3 1.727e-008 1.729e-008 -7.763 -7.762 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

NaCO3- 2.791e-010 2.579e-010 -9.554 -9.588 -0.034

NaOH 1.011e-012 1.013e-012 -11.995 -11.995 0.001

O(0) 3.995e-004

O2 1.997e-004 2.000e-004 -3.700 -3.699 0.001

S(6) 1.154e-004

SO4-2 9.775e-005 7.169e-005 -4.010 -4.145 -0.135

CaSO4 1.255e-005 1.257e-005 -4.901 -4.901 0.001

MgSO4 5.071e-006 5.077e-006 -5.295 -5.294 0.001

NaSO4- 3.422e-009 3.163e-009 -8.466 -8.500 -0.034

KSO4- 1.466e-009 1.354e-009 -8.834 -8.868 -0.034

HSO4- 3.886e-010 3.592e-010 -9.410 -9.445 -0.034

CaHSO4+ 4.406e-012 4.072e-012 -11.356 -11.390 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.39 -8.68 -8.29 CaCO3

Calcite -0.24 -8.68 -8.44 CaCO3

CO2(g) -1.92 -3.30 -1.38 CO2

Dolomite -0.86 -17.78 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.44 -25.56 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.86 -3.70 -2.83 O2

Initial solution 120. 30/8/2012 17:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.672e-003 3.672e-003

Ca 1.339e-003 1.339e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.857e-004 3.857e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.200

pe = 4.000

Specific Conductance (uS/cm, 17 oC) = 296

Density (g/cm3) = 0.99892

Activity of water = 1.000

Ionic strength = 5.633e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 4.192e-003

Total CO2 (mol/kg) = 4.192e-003

Temperature (deg C) = 17.600

Electrical balance (eq) = -2.308e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.08

Iterations = 7

Total H = 1.110161e+002

Total O = 5.551911e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 14.0201 0.8088

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.602e-008 8.863e-008 -7.018 -7.052 -0.035

H+ 6.775e-008 6.310e-008 -7.169 -7.200 -0.031

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 4.192e-003

HCO3- 3.606e-003 3.339e-003 -2.443 -2.476 -0.033

CO2 5.270e-004 5.277e-004 -3.278 -3.278 0.001

CaHCO3+ 3.809e-005 3.528e-005 -4.419 -4.452 -0.033

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

CaCO3 2.941e-006 2.944e-006 -5.532 -5.531 0.001

CO3-2 2.863e-006 2.106e-006 -5.543 -5.676 -0.133

MgCO3 6.579e-007 6.587e-007 -6.182 -6.181 0.001

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaCO3- 2.673e-010 2.470e-010 -9.573 -9.607 -0.034

Ca 1.339e-003

Ca+2 1.286e-003 9.453e-004 -2.891 -3.024 -0.134

CaHCO3+ 3.809e-005 3.528e-005 -4.419 -4.452 -0.033

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

CaCO3 2.941e-006 2.944e-006 -5.532 -5.531 0.001

CaOH+ 2.690e-009 2.486e-009 -8.570 -8.604 -0.034

CaHSO4+ 4.623e-012 4.272e-012 -11.335 -11.369 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.288e-005 -4.242 -4.277 -0.035

H(0) 6.071e-026

H2 3.036e-026 3.040e-026 -25.518 -25.517 0.001

K 3.326e-006

K+ 3.324e-006 3.069e-006 -5.478 -5.513 -0.035

KSO4- 1.465e-009 1.354e-009 -8.834 -8.869 -0.034

KOH 1.684e-013 1.686e-013 -12.774 -12.773 0.001

Mg 5.184e-004

Mg+2 4.976e-004 3.672e-004 -3.303 -3.435 -0.132

MgHCO3+ 1.511e-005 1.396e-005 -4.821 -4.855 -0.034

MgSO4 5.066e-006 5.073e-006 -5.295 -5.295 0.001

MgCO3 6.579e-007 6.587e-007 -6.182 -6.181 0.001

MgOH+ 1.152e-008 1.065e-008 -7.938 -7.973 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.235e-006 -5.001 -5.035 -0.034

NaHCO3 1.732e-008 1.734e-008 -7.761 -7.761 0.001

NaSO4- 3.420e-009 3.161e-009 -8.466 -8.500 -0.034

NaCO3- 2.673e-010 2.470e-010 -9.573 -9.607 -0.034

NaOH 9.657e-013 9.669e-013 -12.015 -12.015 0.001

O(0) 3.857e-004

O2 1.929e-004 1.931e-004 -3.715 -3.714 0.001

S(6) 1.154e-004

SO4-2 9.773e-005 7.166e-005 -4.010 -4.145 -0.135

CaSO4 1.257e-005 1.259e-005 -4.901 -4.900 0.001

MgSO4 5.066e-006 5.073e-006 -5.295 -5.295 0.001

NaSO4- 3.420e-009 3.161e-009 -8.466 -8.500 -0.034

KSO4- 1.465e-009 1.354e-009 -8.834 -8.869 -0.034

HSO4- 4.068e-010 3.759e-010 -9.391 -9.425 -0.034

CaHSO4+ 4.623e-012 4.272e-012 -11.335 -11.369 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.83 -7.17 -4.34 CaSO4

Aragonite -0.41 -8.70 -8.29 CaCO3

Calcite -0.26 -8.70 -8.44 CaCO3

CO2(g) -1.90 -3.28 -1.38 CO2

Dolomite -0.90 -17.81 -16.91 CaMg(CO3)2

Gypsum -2.59 -7.17 -4.58 CaSO4:2H2O

H2(g) -22.40 -25.52 -3.12 H2

H2O(g) -1.71 -0.00 1.71 H2O

Halite -10.88 -9.31 1.56 NaCl

O2(g) -0.88 -3.71 -2.83 O2

------------------

End of simulation.

------------------

------------------------------------

Reading input data for simulation 2.

------------------------------------

-----------

End of run.

Input file: C:\Users\huan\Desktop\Maolan midstream.pqi

Output file: C:\Users\huan\Desktop\Maolan midstream.pqo

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

------------------

Reading data base.

------------------

SOLUTION\_MASTER\_SPECIES

SOLUTION\_SPECIES

PHASES

EXCHANGE\_MASTER\_SPECIES

EXCHANGE\_SPECIES

SURFACE\_MASTER\_SPECIES

SURFACE\_SPECIES

RATES

END

------------------------------------

Reading input data for simulation 1.

------------------------------------

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

SOLUTION\_SPREAD

units mg/l

Description Number pH Temp O(0) Ca K Mg Na S(6) Cl Alkalinity

mg/L mg/L mg/L mg/L mg/L mg/L mg/L mg/L as HCO3

29/8/2012 11:54:20 1 8.7 27.12 9.98 46.91999817 0.13 12.60 0.23 11.07999992 2.029999971 195.6300049

29/8/2012 12:09:20 2 8.81 27.45 9.13 47.06999969 0.13 12.60 0.23 11.07999992 2.029999971 196.2700043

29/8/2012 12:24:20 3 9 27.86 11.9 47.22000122 0.13 12.60 0.23 11.07999992 2.029999971 196.8899994

29/8/2012 12:39:20 4 9.18 28.34 13.72 47.22000122 0.13 12.60 0.23 11.07999992 2.029999971 196.8899994

29/8/2012 12:54:20 5 9.12 28.81 13.41 47.36999893 0.13 12.60 0.23 11.07999992 2.029999971 197.5200043

29/8/2012 13:09:20 6 9.05 29.28 12.86 46.77000046 0.13 12.60 0.23 11.07999992 2.029999971 195

29/8/2012 13:24:20 7 9.06 29.68 14.15 47.06999969 0.13 12.60 0.23 11.07999992 2.029999971 196.2700043

29/8/2012 13:39:20 8 9.05 30.07 14.86 46.91999817 0.13 12.60 0.23 11.07999992 2.029999971 195.6300049

29/8/2012 13:54:20 9 9.03 30.33 14.89 46.47000122 0.13 12.60 0.23 11.07999992 2.029999971 193.75

29/8/2012 14:09:20 10 9.03 30.62 14.86 46.61999893 0.13 12.60 0.23 11.07999992 2.029999971 194.3800049

29/8/2012 14:24:20 11 8.98 30.76 15.08 46.61999893 0.13 12.60 0.23 11.07999992 2.029999971 194.3800049

29/8/2012 14:39:20 12 8.96 30.91 15.19 46.16999817 0.13 12.60 0.23 11.07999992 2.029999971 192.4900055

29/8/2012 14:54:20 13 9.05 31.12 15.53 43.77000046 0.13 12.60 0.23 11.07999992 2.029999971 182.4100037

29/8/2012 15:09:20 14 9.06 31.22 15.63 43.77000046 0.13 12.60 0.23 11.07999992 2.029999971 182.4100037

29/8/2012 15:24:20 15 9.06 31.22 15.9 43.77000046 0.13 12.60 0.23 11.07999992 2.029999971 182.4100037

29/8/2012 15:39:20 16 9.06 31.17 15.92 43.31999969 0.13 12.60 0.23 11.07999992 2.029999971 180.5200043

29/8/2012 15:54:20 17 9.06 31.07 15.92 43.02000046 0.13 12.60 0.23 11.07999992 2.029999971 179.25

29/8/2012 16:09:20 18 9.05 30.87 15.93 42.56999969 0.13 12.60 0.23 11.07999992 2.029999971 177.3600006

29/8/2012 16:24:20 19 9.1 30.76 16.15 41.97000122 0.13 12.60 0.23 11.07999992 2.029999971 174.8500061

29/8/2012 16:39:20 20 9.14 30.59 16.06 41.22000122 0.13 12.60 0.23 11.07999992 2.029999971 171.6900024

29/8/2012 16:54:20 21 9.2 30.53 16.06 40.61999893 0.13 12.60 0.23 11.07999992 2.029999971 169.1699982

29/8/2012 17:09:20 22 9.21 30.39 16.08 40.61999893 0.13 12.60 0.23 11.07999992 2.029999971 169.1699982

29/8/2012 17:24:20 23 9.24 30.2 16.14 40.77000046 0.13 12.60 0.23 11.07999992 2.029999971 169.8000031

29/8/2012 17:39:20 24 9.25 30.03 16.43 40.77000046 0.13 12.60 0.23 11.07999992 2.029999971 169.8000031

29/8/2012 17:54:20 25 9.28 29.81 16.01 40.61999893 0.13 12.60 0.23 11.07999992 2.029999971 169.1699982

29/8/2012 18:09:20 26 9.31 29.63 15.91 40.02000046 0.13 12.60 0.23 11.07999992 2.029999971 166.6600037

29/8/2012 18:24:20 27 9.28 29.42 15.83 40.02000046 0.13 12.60 0.23 11.07999992 2.029999971 166.6600037

29/8/2012 18:39:20 28 9.25 29.2 15.78 40.31999969 0.13 12.60 0.23 11.07999992 2.029999971 167.9100037

29/8/2012 18:54:20 29 9.21 29.02 15.7 40.31999969 0.13 12.60 0.23 11.07999992 2.029999971 167.9100037

29/8/2012 19:09:20 30 9.13 28.76 15.61 40.61999893 0.13 12.60 0.23 11.07999992 2.029999971 169.1699982

29/8/2012 19:24:20 31 9.11 28.57 15.52 40.61999893 0.13 12.60 0.23 11.07999992 2.029999971 169.1699982

29/8/2012 19:39:20 32 9.03 28.36 15.37 40.77000046 0.13 12.60 0.23 11.07999992 2.029999971 169.8000031

29/8/2012 19:54:20 33 8.95 28.16 15.22 41.22000122 0.13 12.60 0.23 11.07999992 2.029999971 171.6900024

29/8/2012 20:09:20 34 8.91 28 15.04 41.22000122 0.13 12.60 0.23 11.07999992 2.029999971 171.6900024

29/8/2012 20:24:20 35 8.83 27.85 14.86 41.36999893 0.13 12.60 0.23 11.07999992 2.029999971 172.3300018

29/8/2012 20:39:20 36 8.73 27.69 14.64 41.66999817 0.13 12.60 0.23 11.07999992 2.029999971 173.5800018

29/8/2012 20:54:20 37 8.71 27.54 14.29 42.27000046 0.13 12.60 0.23 11.07999992 2.029999971 176.1100006

29/8/2012 21:09:20 38 8.67 27.43 14.02 42.41999817 0.13 12.60 0.23 11.07999992 2.029999971 176.7400055

29/8/2012 21:24:20 39 8.61 27.3 13.71 42.56999969 0.13 12.60 0.23 11.07999992 2.029999971 177.3600006

29/8/2012 21:39:20 40 8.56 27.22 13.37 42.72000122 0.13 12.60 0.23 11.07999992 2.029999971 178

29/8/2012 21:54:20 41 8.49 27.1 13.08 43.02000046 0.13 12.60 0.23 11.07999992 2.029999971 179.25

29/8/2012 22:09:20 42 8.43 26.99 12.69 43.31999969 0.13 12.60 0.23 11.07999992 2.029999971 180.5200043

29/8/2012 22:24:20 43 8.35 26.88 12.16 43.61999893 0.13 12.60 0.23 11.07999992 2.029999971 181.7700043

29/8/2012 22:39:20 44 8.25 26.76 11.87 43.77000046 0.13 12.60 0.23 11.07999992 2.029999971 182.4100037

29/8/2012 22:54:20 45 8.19 26.65 11.49 43.77000046 0.13 12.60 0.23 11.07999992 2.029999971 182.4100037

29/8/2012 23:09:20 46 8.13 26.55 11.1 44.06999969 0.13 12.60 0.23 11.07999992 2.029999971 183.6600037

29/8/2012 23:24:20 47 8.09 26.45 10.69 44.22000122 0.13 12.60 0.23 11.07999992 2.029999971 184.3000031

29/8/2012 23:39:20 48 8.05 26.36 9.89 44.36999893 0.13 12.60 0.23 11.07999992 2.029999971 184.9199982

29/8/2012 23:54:20 49 7.99 26.27 9.47 44.66999817 0.13 12.60 0.23 11.07999992 2.029999971 186.1900024

30/8/2012 00:09:20 50 7.94 26.31 9.03 44.81999969 0.13 12.60 0.23 11.07999992 2.029999971 186.8200073

30/8/2012 00:24:20 51 7.89 26.18 8.62 44.81999969 0.13 12.60 0.23 11.07999992 2.029999971 186.8200073

30/8/2012 00:39:20 52 7.85 26.18 8.24 45.11999893 0.13 12.60 0.23 11.07999992 2.029999971 188.0800018

30/8/2012 00:54:20 53 7.82 25.96 7.88 45.41999817 0.13 12.60 0.23 11.07999992 2.029999971 189.3300018

30/8/2012 01:09:20 54 7.77 25.92 7.47 45.41999817 0.13 12.60 0.23 11.07999992 2.029999971 189.3300018

30/8/2012 01:24:20 55 7.76 25.82 7.03 45.72000122 0.13 12.60 0.23 11.07999992 2.029999971 190.6000061

30/8/2012 01:39:20 56 7.71 25.76 5.52 45.86999893 0.13 12.60 0.23 11.07999992 2.029999971 191.2200012

30/8/2012 01:54:20 57 7.7 25.67 5.01 46.02000046 0.13 12.60 0.23 11.07999992 2.029999971 191.8600006

30/8/2012 02:09:20 58 7.66 25.61 4.45 46.02000046 0.13 12.60 0.23 11.07999992 2.029999971 191.8600006

30/8/2012 02:24:20 59 7.65 25.57 4.24 46.31999969 0.13 12.60 0.23 11.07999992 2.029999971 193.1100006

30/8/2012 02:39:20 60 7.63 25.48 3.77 46.47000122 0.13 12.60 0.23 11.07999992 2.029999971 193.75

30/8/2012 02:54:20 61 7.61 25.41 3.59 46.77000046 0.13 12.60 0.23 11.07999992 2.029999971 195

30/8/2012 03:09:20 62 7.59 25.38 3.06 46.91999817 0.13 12.60 0.23 11.07999992 2.029999971 195.6300049

30/8/2012 03:24:20 63 7.56 25.33 2.72 47.06999969 0.13 12.60 0.23 11.07999992 2.029999971 196.2700043

30/8/2012 03:39:20 64 7.55 25.26 2.33 47.22000122 0.13 12.60 0.23 11.07999992 2.029999971 196.8899994

30/8/2012 03:54:20 65 7.55 25.2 2.08 47.52000046 0.13 12.60 0.23 11.07999992 2.029999971 198.1600037

30/8/2012 04:09:20 66 7.53 25.13 1.71 47.66999817 0.13 12.60 0.23 11.07999992 2.029999971 198.7799988

30/8/2012 04:24:20 67 7.52 25.05 1.15 47.81999969 0.13 12.60 0.23 11.07999992 2.029999971 199.4100037

30/8/2012 04:39:20 68 7.5 25.02 0.64 47.81999969 0.13 12.60 0.23 11.07999992 2.029999971 199.4100037

30/8/2012 04:54:20 69 7.48 24.96 0.42 47.97000122 0.13 12.60 0.23 11.07999992 2.029999971 200.0500031

30/8/2012 05:09:20 70 7.47 24.88 0.31 47.97000122 0.13 12.60 0.23 11.07999992 2.029999971 200.0500031

30/8/2012 05:24:20 71 7.47 24.82 0.18 48.11999893 0.13 12.60 0.23 11.07999992 2.029999971 200.6699982

30/8/2012 05:39:20 72 7.48 24.75 0.13 48.27000046 0.13 12.60 0.23 11.07999992 2.029999971 201.3000031

30/8/2012 05:54:20 73 7.48 24.7 0.09 48.27000046 0.13 12.60 0.23 11.07999992 2.029999971 201.3000031

30/8/2012 06:09:20 74 7.48 24.62 0.07 48.41999817 0.13 12.60 0.23 11.07999992 2.029999971 201.9400024

30/8/2012 06:24:20 75 7.49 24.57 0.05 48.56999969 0.13 12.60 0.23 11.07999992 2.029999971 202.5700073

30/8/2012 06:39:20 76 7.48 24.5 0.05 48.86999893 0.13 12.60 0.23 11.07999992 2.029999971 203.8300018

30/8/2012 06:54:20 77 7.48 24.45 0.09 48.86999893 0.13 12.60 0.23 11.07999992 2.029999971 203.8300018

30/8/2012 07:09:20 78 7.48 24.36 0.12 49.02000046 0.13 12.60 0.23 11.07999992 2.029999971 204.4600067

30/8/2012 07:24:20 79 7.48 24.31 0.09 49.02000046 0.13 12.60 0.23 11.07999992 2.029999971 204.4600067

30/8/2012 07:39:20 80 7.48 24.24 0.07 49.31999969 0.13 12.60 0.23 11.07999992 2.029999971 205.7200012

30/8/2012 07:54:20 81 7.49 24.24 0.25 49.31999969 0.13 12.60 0.23 11.07999992 2.029999971 205.7200012

30/8/2012 08:09:20 82 7.5 24.31 0.37 49.47000122 0.13 12.60 0.23 11.07999992 2.029999971 206.3500061

30/8/2012 08:24:20 83 7.53 24.35 0.65 49.47000122 0.13 12.60 0.23 11.07999992 2.029999971 206.3500061

30/8/2012 08:39:20 84 7.54 24.38 0.61 49.47000122 0.13 12.60 0.23 11.07999992 2.029999971 206.3500061

30/8/2012 08:54:20 85 7.57 24.52 0.67 49.31999969 0.13 12.60 0.23 11.07999992 2.029999971 205.7200012

30/8/2012 09:09:20 86 7.61 24.68 1.39 49.31999969 0.13 12.60 0.23 11.07999992 2.029999971 205.7200012

30/8/2012 09:24:20 87 7.66 24.83 2.49 49.31999969 0.13 12.60 0.23 11.07999992 2.029999971 205.7200012

30/8/2012 09:39:20 88 7.75 24.93 3.98 49.16999817 0.13 12.60 0.23 11.07999992 2.029999971 205.0800018

30/8/2012 09:54:20 89 7.85 25.03 5.2 49.02000046 0.13 12.60 0.23 11.07999992 2.029999971 204.4600067

30/8/2012 10:09:20 90 8.04 25.03 6.28 48.72000122 0.13 12.60 0.23 11.07999992 2.029999971 203.1900024

30/8/2012 10:24:20 91 8.11 25.36 7 48.56999969 0.13 12.60 0.23 11.07999992 2.029999971 202.5700073

30/8/2012 10:39:20 92 8.26 25.58 7.79 48.41999817 0.13 12.60 0.23 11.07999992 2.029999971 201.9400024

30/8/2012 10:54:20 93 8.37 25.92 8.87 48.41999817 0.13 12.60 0.23 11.07999992 2.029999971 201.9400024

30/8/2012 11:09:20 94 8.37 26.3 10.51 48.41999817 0.13 12.60 0.23 11.07999992 2.029999971 201.9400024

30/8/2012 11:24:20 95 8.64 26.84 11.32 48.41999817 0.13 12.60 0.23 11.07999992 2.029999971 201.9400024

30/8/2012 11:39:20 96 8.86 27.32 13.16 48.27000046 0.13 12.60 0.23 11.07999992 2.029999971 201.3000031

30/8/2012 11:54:20 97 8.96 27.78 15.09 47.97000122 0.13 12.60 0.23 11.07999992 2.029999971 200.0500031

30/8/2012 12:09:20 98 8.98 28.3 15.68 47.81999969 0.13 12.60 0.23 11.07999992 2.029999971 199.4100037

30/8/2012 12:24:20 99 9.09 28.73 17.23 47.22000122 0.13 12.60 0.23 11.07999992 2.029999971 196.8899994

30/8/2012 12:39:20 100 9.08 29.32 19.2 47.22000122 0.13 12.60 0.23 11.07999992 2.029999971 196.8899994

30/8/2012 12:54:20 101 9.05 29.75 18.98 46.61999893 0.13 12.60 0.23 11.07999992 2.029999971 194.3800049

30/8/2012 13:09:20 102 9.04 30.14 20.02 45.86999893 0.13 12.60 0.23 11.07999992 2.029999971 191.2200012

30/8/2012 13:24:20 103 9.04 30.49 19.97 44.97000122 0.13 12.60 0.23 11.07999992 2.029999971 187.4400024

30/8/2012 13:39:20 104 9.05 30.61 22.56 44.22000122 0.13 12.60 0.23 11.07999992 2.029999971 184.3000031

30/8/2012 13:54:20 105 9.08 30.68 22.56 43.47000122 0.13 12.60 0.23 11.07999992 2.029999971 181.1399994

30/8/2012 14:09:20 106 9.08 30.95 23.49 43.16999817 0.13 12.60 0.23 11.07999992 2.029999971 179.8800049

30/8/2012 14:24:20 107 9.08 31.18 21.11 43.02000046 0.13 12.60 0.23 11.07999992 2.029999971 179.25

30/8/2012 14:54:20 108 9.12 31.4 21.1 42.41999817 0.13 12.60 0.23 11.07999992 2.029999971 176.7400055

30/8/2012 15:09:20 109 9.16 31.52 21.65 41.66999817 0.13 12.60 0.23 11.07999992 2.029999971 173.5800018

30/8/2012 15:24:20 110 9.15 31.65 21.35 41.97000122 0.13 12.60 0.23 11.07999992 2.029999971 174.8500061

30/8/2012 15:39:20 111 9.17 31.74 21.99 41.52000046 0.13 12.60 0.23 11.07999992 2.029999971 172.9600067

30/8/2012 15:54:20 112 9.14 31.78 21.8 41.52000046 0.13 12.60 0.23 11.07999992 2.029999971 172.9600067

30/8/2012 16:09:20 113 9.15 31.79 21.31 41.22000122 0.13 12.60 0.23 11.07999992 2.029999971 171.6900024

30/8/2012 16:24:20 114 9.15 31.74 21.65 40.61999893 0.13 12.60 0.23 11.07999992 2.029999971 169.1699982

30/8/2012 16:39:20 115 9.2 31.53 21.69 40.02000046 0.13 12.60 0.23 11.07999992 2.029999971 166.6600037

30/8/2012 16:54:20 116 9.18 31.21 21.27 39.56999969 0.13 12.60 0.23 11.07999992 2.029999971 164.7700043

30/8/2012 17:09:20 117 9.24 30.86 21.37 37.47000122 0.13 12.60 0.23 11.07999992 2.029999971 155.9400024

30/8/2012 17:24:20 118 9.52 30.56 19.14 36.72000122 0.13 12.60 0.23 11.07999992 2.029999971 152.8000031

30/8/2012 17:39:20 119 9.62 30.33 19.02 36.56999969 0.13 12.60 0.23 11.07999992 2.029999971 152.1600037

30/8/2012 17:54:20 120 9.54 30.13 19.01 36.56999969 0.13 12.60 0.23 11.07999992 2.029999971 152.1600037

SELECTED\_OUTPUT

file C:\Users\huan\Desktop\selected output midstream.sel

reset false

saturation\_indices Calcite CO2(g)

-------------------------------------------

Beginning of initial solution calculations.

-------------------------------------------

Initial solution 1. 29/8/2012 11:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.207e-003 3.207e-003

Ca 1.171e-003 1.171e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.239e-004 6.239e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.700

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 319

Density (g/cm3) = 0.99670

Activity of water = 1.000

Ionic strength = 4.853e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.018e-003

Total CO2 (mol/kg) = 3.018e-003

Temperature (deg C) = 27.120

Electrical balance (eq) = -1.028e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.63

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551635e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.7693 0.7012

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 6.343e-006 5.879e-006 -5.198 -5.231 -0.033

H+ 2.136e-009 1.995e-009 -8.670 -8.700 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.018e-003

HCO3- 2.773e-003 2.578e-003 -2.557 -2.589 -0.032

CaCO3 8.637e-005 8.647e-005 -4.064 -4.063 0.000

CO3-2 8.457e-005 6.316e-005 -4.073 -4.200 -0.127

CaHCO3+ 2.845e-005 2.645e-005 -4.546 -4.578 -0.032

MgCO3 2.223e-005 2.225e-005 -4.653 -4.653 0.000

MgHCO3+ 1.173e-005 1.089e-005 -4.931 -4.963 -0.033

CO2 1.127e-005 1.128e-005 -4.948 -4.948 0.000

NaHCO3 1.341e-008 1.343e-008 -7.872 -7.872 0.000

NaCO3- 1.306e-008 1.212e-008 -7.884 -7.917 -0.033

Ca 1.171e-003

Ca+2 1.045e-003 7.797e-004 -2.981 -3.108 -0.127

CaCO3 8.637e-005 8.647e-005 -4.064 -4.063 0.000

CaHCO3+ 2.845e-005 2.645e-005 -4.546 -4.578 -0.032

CaSO4 1.150e-005 1.152e-005 -4.939 -4.939 0.000

CaOH+ 6.990e-008 6.485e-008 -7.156 -7.188 -0.033

CaHSO4+ 1.490e-013 1.383e-013 -12.827 -12.859 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.310e-005 -4.242 -4.275 -0.033

H(0) 5.514e-029

H2 2.757e-029 2.760e-029 -28.560 -28.559 0.000

K 3.326e-006

K+ 3.324e-006 3.081e-006 -5.478 -5.511 -0.033

KSO4- 1.757e-009 1.630e-009 -8.755 -8.788 -0.033

KOH 5.348e-012 5.354e-012 -11.272 -11.271 0.000

Mg 5.184e-004

Mg+2 4.772e-004 3.574e-004 -3.321 -3.447 -0.126

MgCO3 2.223e-005 2.225e-005 -4.653 -4.653 0.000

MgHCO3+ 1.173e-005 1.089e-005 -4.931 -4.963 -0.033

MgSO4 6.412e-006 6.419e-006 -5.193 -5.193 0.000

MgOH+ 8.476e-007 7.864e-007 -6.072 -6.104 -0.033

Na 1.001e-005

Na+ 9.977e-006 9.263e-006 -5.001 -5.033 -0.032

NaHCO3 1.341e-008 1.343e-008 -7.872 -7.872 0.000

NaCO3- 1.306e-008 1.212e-008 -7.884 -7.917 -0.033

NaSO4- 3.680e-009 3.415e-009 -8.434 -8.467 -0.033

NaOH 3.064e-011 3.067e-011 -10.514 -10.513 0.000

O(0) 6.239e-004

O2 3.120e-004 3.123e-004 -3.506 -3.505 0.000

S(6) 1.154e-004

SO4-2 9.745e-005 7.258e-005 -4.011 -4.139 -0.128

CaSO4 1.150e-005 1.152e-005 -4.939 -4.939 0.000

MgSO4 6.412e-006 6.419e-006 -5.193 -5.193 0.000

NaSO4- 3.680e-009 3.415e-009 -8.434 -8.467 -0.033

KSO4- 1.757e-009 1.630e-009 -8.755 -8.788 -0.033

HSO4- 1.590e-011 1.475e-011 -10.799 -10.831 -0.033

CaHSO4+ 1.490e-013 1.383e-013 -12.827 -12.859 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 1.04 -7.31 -8.35 CaCO3

Calcite 1.18 -7.31 -8.49 CaCO3

CO2(g) -3.46 -4.95 -1.49 CO2

Dolomite 2.18 -14.95 -17.14 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -25.40 -28.56 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.60 -3.51 -2.91 O2

Initial solution 2. 29/8/2012 12:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.217e-003 3.217e-003

Ca 1.175e-003 1.175e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.708e-004 5.708e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.810

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 318

Density (g/cm3) = 0.99661

Activity of water = 1.000

Ionic strength = 4.810e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.975e-003

Total CO2 (mol/kg) = 2.975e-003

Temperature (deg C) = 27.450

Electrical balance (eq) = -1.058e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.70

Iterations = 7

Total H = 1.110152e+002

Total O = 5.551617e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.6227 0.6932

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.370e-006 7.761e-006 -5.077 -5.110 -0.033

H+ 1.657e-009 1.549e-009 -8.781 -8.810 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.975e-003

HCO3- 2.686e-003 2.498e-003 -2.571 -2.602 -0.032

CaCO3 1.077e-004 1.078e-004 -3.968 -3.967 0.000

CO3-2 1.061e-004 7.933e-005 -3.974 -4.101 -0.126

MgCO3 2.778e-005 2.781e-005 -4.556 -4.556 0.000

CaHCO3+ 2.728e-005 2.537e-005 -4.564 -4.596 -0.032

MgHCO3+ 1.127e-005 1.046e-005 -4.948 -4.981 -0.032

CO2 8.445e-006 8.454e-006 -5.073 -5.073 0.000

NaCO3- 1.667e-008 1.547e-008 -7.778 -7.811 -0.032

NaHCO3 1.300e-008 1.301e-008 -7.886 -7.886 0.000

Ca 1.175e-003

Ca+2 1.028e-003 7.683e-004 -2.988 -3.114 -0.127

CaCO3 1.077e-004 1.078e-004 -3.968 -3.967 0.000

CaHCO3+ 2.728e-005 2.537e-005 -4.564 -4.596 -0.032

CaSO4 1.139e-005 1.141e-005 -4.943 -4.943 0.000

CaOH+ 8.870e-008 8.232e-008 -7.052 -7.084 -0.032

CaHSO4+ 1.151e-013 1.068e-013 -12.939 -12.972 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.311e-005 -4.242 -4.275 -0.033

H(0) 3.312e-029

H2 1.656e-029 1.658e-029 -28.781 -28.781 0.000

K 3.326e-006

K+ 3.324e-006 3.082e-006 -5.478 -5.511 -0.033

KSO4- 1.771e-009 1.643e-009 -8.752 -8.784 -0.032

KOH 6.892e-012 6.900e-012 -11.162 -11.161 0.000

Mg 5.184e-004

Mg+2 4.718e-004 3.537e-004 -3.326 -3.451 -0.125

MgCO3 2.778e-005 2.781e-005 -4.556 -4.556 0.000

MgHCO3+ 1.127e-005 1.046e-005 -4.948 -4.981 -0.032

MgSO4 6.413e-006 6.420e-006 -5.193 -5.192 0.000

MgOH+ 1.113e-006 1.033e-006 -5.954 -5.986 -0.032

Na 1.001e-005

Na+ 9.974e-006 9.262e-006 -5.001 -5.033 -0.032

NaCO3- 1.667e-008 1.547e-008 -7.778 -7.811 -0.032

NaHCO3 1.300e-008 1.301e-008 -7.886 -7.886 0.000

NaSO4- 3.694e-009 3.429e-009 -8.432 -8.465 -0.032

NaOH 3.946e-011 3.951e-011 -10.404 -10.403 0.000

O(0) 5.708e-004

O2 2.854e-004 2.857e-004 -3.545 -3.544 0.000

S(6) 1.154e-004

SO4-2 9.756e-005 7.273e-005 -4.011 -4.138 -0.128

CaSO4 1.139e-005 1.141e-005 -4.943 -4.943 0.000

MgSO4 6.413e-006 6.420e-006 -5.193 -5.192 0.000

NaSO4- 3.694e-009 3.429e-009 -8.432 -8.465 -0.032

KSO4- 1.771e-009 1.643e-009 -8.752 -8.784 -0.032

HSO4- 1.246e-011 1.156e-011 -10.905 -10.937 -0.032

CaHSO4+ 1.151e-013 1.068e-013 -12.939 -12.972 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 1.14 -7.21 -8.35 CaCO3

Calcite 1.28 -7.21 -8.49 CaCO3

CO2(g) -3.58 -5.07 -1.50 CO2

Dolomite 2.38 -14.77 -17.15 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -25.62 -28.78 -3.16 H2

H2O(g) -1.45 -0.00 1.45 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.63 -3.54 -2.91 O2

Initial solution 3. 29/8/2012 12:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.228e-003 3.228e-003

Ca 1.178e-003 1.178e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 7.440e-004 7.440e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.000

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 314

Density (g/cm3) = 0.99650

Activity of water = 1.000

Ionic strength = 4.709e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.873e-003

Total CO2 (mol/kg) = 2.873e-003

Temperature (deg C) = 27.860

Electrical balance (eq) = -1.085e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.80

Iterations = 7

Total H = 1.110150e+002

Total O = 5.551605e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.4281 0.6825

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.335e-005 1.239e-005 -4.874 -4.907 -0.033

H+ 1.070e-009 1.000e-009 -8.971 -9.000 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.873e-003

HCO3- 2.488e-003 2.315e-003 -2.604 -2.635 -0.031

CO3-2 1.531e-004 1.148e-004 -3.815 -3.940 -0.125

CaCO3 1.518e-004 1.520e-004 -3.819 -3.818 0.000

MgCO3 3.957e-005 3.961e-005 -4.403 -4.402 0.000

CaHCO3+ 2.455e-005 2.284e-005 -4.610 -4.641 -0.031

MgHCO3+ 1.023e-005 9.504e-006 -4.990 -5.022 -0.032

CO2 5.032e-006 5.038e-006 -5.298 -5.298 0.000

NaCO3- 2.459e-008 2.284e-008 -7.609 -7.641 -0.032

NaHCO3 1.205e-008 1.206e-008 -7.919 -7.919 0.000

Ca 1.178e-003

Ca+2 9.908e-004 7.422e-004 -3.004 -3.129 -0.125

CaCO3 1.518e-004 1.520e-004 -3.819 -3.818 0.000

CaHCO3+ 2.455e-005 2.284e-005 -4.610 -4.641 -0.031

CaSO4 1.111e-005 1.112e-005 -4.954 -4.954 0.000

CaOH+ 1.326e-007 1.232e-007 -6.877 -6.910 -0.032

CaHSO4+ 7.280e-014 6.760e-014 -13.138 -13.170 -0.032

Cl 5.728e-005

Cl- 5.728e-005 5.315e-005 -4.242 -4.275 -0.032

H(0) 1.375e-029

H2 6.875e-030 6.883e-030 -29.163 -29.162 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.794e-009 1.666e-009 -8.746 -8.778 -0.032

KOH 1.068e-011 1.069e-011 -10.971 -10.971 0.000

Mg 5.184e-004

Mg+2 4.605e-004 3.461e-004 -3.337 -3.461 -0.124

MgCO3 3.957e-005 3.961e-005 -4.403 -4.402 0.000

MgHCO3+ 1.023e-005 9.504e-006 -4.990 -5.022 -0.032

MgSO4 6.377e-006 6.384e-006 -5.195 -5.195 0.000

MgOH+ 1.747e-006 1.623e-006 -5.758 -5.790 -0.032

Na 1.001e-005

Na+ 9.967e-006 9.262e-006 -5.001 -5.033 -0.032

NaCO3- 2.459e-008 2.284e-008 -7.609 -7.641 -0.032

NaHCO3 1.205e-008 1.206e-008 -7.919 -7.919 0.000

NaSO4- 3.723e-009 3.457e-009 -8.429 -8.461 -0.032

NaOH 6.112e-011 6.119e-011 -10.214 -10.213 0.000

O(0) 7.440e-004

O2 3.720e-004 3.724e-004 -3.429 -3.429 0.000

S(6) 1.154e-004

SO4-2 9.788e-005 7.315e-005 -4.009 -4.136 -0.126

CaSO4 1.111e-005 1.112e-005 -4.954 -4.954 0.000

MgSO4 6.377e-006 6.384e-006 -5.195 -5.195 0.000

NaSO4- 3.723e-009 3.457e-009 -8.429 -8.461 -0.032

KSO4- 1.794e-009 1.666e-009 -8.746 -8.778 -0.032

HSO4- 8.158e-012 7.576e-012 -11.088 -11.121 -0.032

CaHSO4+ 7.280e-014 6.760e-014 -13.138 -13.170 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.27 -4.37 CaSO4

Aragonite 1.29 -7.07 -8.35 CaCO3

Calcite 1.43 -7.07 -8.50 CaCO3

CO2(g) -3.80 -5.30 -1.50 CO2

Dolomite 2.69 -14.47 -17.16 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -26.00 -29.16 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.52 -3.43 -2.91 O2

Initial solution 4. 29/8/2012 12:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.228e-003 3.228e-003

Ca 1.178e-003 1.178e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 8.577e-004 8.577e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.180

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 309

Density (g/cm3) = 0.99636

Activity of water = 1.000

Ionic strength = 4.583e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.741e-003

Total CO2 (mol/kg) = 2.741e-003

Temperature (deg C) = 28.340

Electrical balance (eq) = -1.085e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.88

Iterations = 7

Total H = 1.110147e+002

Total O = 5.551578e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.2246 0.6714

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.091e-005 1.942e-005 -4.680 -4.712 -0.032

H+ 7.061e-010 6.607e-010 -9.151 -9.180 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.741e-003

HCO3- 2.242e-003 2.088e-003 -2.649 -2.680 -0.031

CO3-2 2.102e-004 1.581e-004 -3.677 -3.801 -0.124

CaCO3 2.020e-004 2.022e-004 -3.695 -3.694 0.000

MgCO3 5.344e-005 5.350e-005 -4.272 -4.272 0.000

CaHCO3+ 2.128e-005 1.982e-005 -4.672 -4.703 -0.031

MgHCO3+ 9.000e-006 8.365e-006 -5.046 -5.078 -0.032

CO2 2.983e-006 2.986e-006 -5.525 -5.525 0.000

NaCO3- 3.464e-008 3.220e-008 -7.460 -7.492 -0.032

NaHCO3 1.086e-008 1.087e-008 -7.964 -7.964 0.000

Ca 1.178e-003

Ca+2 9.442e-004 7.096e-004 -3.025 -3.149 -0.124

CaCO3 2.020e-004 2.022e-004 -3.695 -3.694 0.000

CaHCO3+ 2.128e-005 1.982e-005 -4.672 -4.703 -0.031

CaSO4 1.075e-005 1.076e-005 -4.969 -4.968 0.000

CaOH+ 1.918e-007 1.782e-007 -6.717 -6.749 -0.032

CaHSO4+ 4.679e-014 4.349e-014 -13.330 -13.362 -0.032

Cl 5.728e-005

Cl- 5.728e-005 5.319e-005 -4.242 -4.274 -0.032

H(0) 5.974e-030

H2 2.987e-030 2.990e-030 -29.525 -29.524 0.000

K 3.326e-006

K+ 3.324e-006 3.087e-006 -5.478 -5.510 -0.032

KSO4- 1.822e-009 1.693e-009 -8.739 -8.771 -0.032

KOH 1.618e-011 1.620e-011 -10.791 -10.791 0.000

Mg 5.184e-004

Mg+2 4.469e-004 3.370e-004 -3.350 -3.472 -0.123

MgCO3 5.344e-005 5.350e-005 -4.272 -4.272 0.000

MgHCO3+ 9.000e-006 8.365e-006 -5.046 -5.078 -0.032

MgSO4 6.332e-006 6.339e-006 -5.198 -5.198 0.000

MgOH+ 2.685e-006 2.495e-006 -5.571 -5.603 -0.032

Na 1.001e-005

Na+ 9.958e-006 9.261e-006 -5.002 -5.033 -0.031

NaCO3- 3.464e-008 3.220e-008 -7.460 -7.492 -0.032

NaHCO3 1.086e-008 1.087e-008 -7.964 -7.964 0.000

NaSO4- 3.759e-009 3.493e-009 -8.425 -8.457 -0.032

NaOH 9.251e-011 9.261e-011 -10.034 -10.033 0.000

O(0) 8.577e-004

O2 4.289e-004 4.293e-004 -3.368 -3.367 0.000

S(6) 1.154e-004

SO4-2 9.828e-005 7.370e-005 -4.008 -4.133 -0.125

CaSO4 1.075e-005 1.076e-005 -4.969 -4.968 0.000

MgSO4 6.332e-006 6.339e-006 -5.198 -5.198 0.000

NaSO4- 3.759e-009 3.493e-009 -8.425 -8.457 -0.032

KSO4- 1.822e-009 1.693e-009 -8.739 -8.771 -0.032

HSO4- 5.484e-012 5.097e-012 -11.261 -11.293 -0.032

CaHSO4+ 4.679e-014 4.349e-014 -13.330 -13.362 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.90 -7.28 -4.38 CaSO4

Aragonite 1.41 -6.95 -8.36 CaCO3

Calcite 1.55 -6.95 -8.50 CaCO3

CO2(g) -4.02 -5.52 -1.51 CO2

Dolomite 2.94 -14.22 -17.17 CaMg(CO3)2

Gypsum -2.70 -7.28 -4.58 CaSO4:2H2O

H2(g) -26.36 -29.52 -3.16 H2

H2O(g) -1.42 -0.00 1.42 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.45 -3.37 -2.92 O2

Initial solution 5. 29/8/2012 12:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.238e-003 3.238e-003

Ca 1.182e-003 1.182e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 8.384e-004 8.384e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.120

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 315

Density (g/cm3) = 0.99623

Activity of water = 1.000

Ionic strength = 4.625e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.790e-003

Total CO2 (mol/kg) = 2.790e-003

Temperature (deg C) = 28.810

Electrical balance (eq) = -1.114e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.90

Iterations = 7

Total H = 1.110148e+002

Total O = 5.551591e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.2441 0.6737

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.886e-005 1.750e-005 -4.725 -4.757 -0.032

H+ 8.110e-010 7.586e-010 -9.091 -9.120 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.790e-003

HCO3- 2.325e-003 2.164e-003 -2.634 -2.665 -0.031

CO3-2 1.917e-004 1.439e-004 -3.717 -3.842 -0.124

CaCO3 1.887e-004 1.889e-004 -3.724 -3.724 0.000

MgCO3 4.937e-005 4.942e-005 -4.307 -4.306 0.000

CaHCO3+ 2.254e-005 2.098e-005 -4.647 -4.678 -0.031

MgHCO3+ 9.421e-006 8.753e-006 -5.026 -5.058 -0.032

CO2 3.533e-006 3.536e-006 -5.452 -5.451 0.000

NaCO3- 3.229e-008 3.000e-008 -7.491 -7.523 -0.032

NaHCO3 1.126e-008 1.127e-008 -7.949 -7.948 0.000

Ca 1.182e-003

Ca+2 9.599e-004 7.203e-004 -3.018 -3.142 -0.125

CaCO3 1.887e-004 1.889e-004 -3.724 -3.724 0.000

CaHCO3+ 2.254e-005 2.098e-005 -4.647 -4.678 -0.031

CaSO4 1.092e-005 1.093e-005 -4.962 -4.961 0.000

CaOH+ 1.696e-007 1.576e-007 -6.771 -6.803 -0.032

CaHSO4+ 5.491e-014 5.101e-014 -13.260 -13.292 -0.032

Cl 5.728e-005

Cl- 5.728e-005 5.317e-005 -4.242 -4.274 -0.032

H(0) 7.840e-030

H2 3.920e-030 3.924e-030 -29.407 -29.406 0.000

K 3.326e-006

K+ 3.324e-006 3.086e-006 -5.478 -5.511 -0.032

KSO4- 1.829e-009 1.699e-009 -8.738 -8.770 -0.032

KOH 1.409e-011 1.410e-011 -10.851 -10.851 0.000

Mg 5.184e-004

Mg+2 4.507e-004 3.394e-004 -3.346 -3.469 -0.123

MgCO3 4.937e-005 4.942e-005 -4.307 -4.306 0.000

MgHCO3+ 9.421e-006 8.753e-006 -5.026 -5.058 -0.032

MgSO4 6.427e-006 6.434e-006 -5.192 -5.192 0.000

MgOH+ 2.455e-006 2.281e-006 -5.610 -5.642 -0.032

Na 1.001e-005

Na+ 9.960e-006 9.260e-006 -5.002 -5.033 -0.032

NaCO3- 3.229e-008 3.000e-008 -7.491 -7.523 -0.032

NaHCO3 1.126e-008 1.127e-008 -7.949 -7.948 0.000

NaSO4- 3.755e-009 3.489e-009 -8.425 -8.457 -0.032

NaOH 8.056e-011 8.064e-011 -10.094 -10.093 0.000

O(0) 8.384e-004

O2 4.192e-004 4.196e-004 -3.378 -3.377 0.000

S(6) 1.154e-004

SO4-2 9.802e-005 7.340e-005 -4.009 -4.134 -0.126

CaSO4 1.092e-005 1.093e-005 -4.962 -4.961 0.000

MgSO4 6.427e-006 6.434e-006 -5.192 -5.192 0.000

NaSO4- 3.755e-009 3.489e-009 -8.425 -8.457 -0.032

KSO4- 1.829e-009 1.699e-009 -8.738 -8.770 -0.032

HSO4- 6.340e-012 5.890e-012 -11.198 -11.230 -0.032

CaHSO4+ 5.491e-014 5.101e-014 -13.260 -13.292 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.90 -7.28 -4.38 CaSO4

Aragonite 1.38 -6.98 -8.36 CaCO3

Calcite 1.52 -6.98 -8.50 CaCO3

CO2(g) -3.94 -5.45 -1.51 CO2

Dolomite 2.88 -14.30 -17.18 CaMg(CO3)2

Gypsum -2.69 -7.28 -4.58 CaSO4:2H2O

H2(g) -26.24 -29.41 -3.17 H2

H2O(g) -1.41 -0.00 1.41 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.46 -3.38 -2.92 O2

Initial solution 6. 29/8/2012 13:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.197e-003 3.197e-003

Ca 1.167e-003 1.167e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 8.040e-004 8.040e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.050

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 319

Density (g/cm3) = 0.99609

Activity of water = 1.000

Ionic strength = 4.625e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.801e-003

Total CO2 (mol/kg) = 2.801e-003

Temperature (deg C) = 29.280

Electrical balance (eq) = -1.000e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.70

Iterations = 7

Total H = 1.110149e+002

Total O = 5.551590e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.2716 0.6764

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.661e-005 1.541e-005 -4.780 -4.812 -0.032

H+ 9.529e-010 8.913e-010 -9.021 -9.050 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.801e-003

HCO3- 2.382e-003 2.217e-003 -2.623 -2.654 -0.031

CO3-2 1.686e-004 1.266e-004 -3.773 -3.898 -0.125

CaCO3 1.685e-004 1.687e-004 -3.773 -3.773 0.000

MgCO3 4.420e-005 4.424e-005 -4.355 -4.354 0.000

CaHCO3+ 2.334e-005 2.172e-005 -4.632 -4.663 -0.031

MgHCO3+ 9.780e-006 9.086e-006 -5.010 -5.042 -0.032

CO2 4.232e-006 4.237e-006 -5.373 -5.373 0.000

NaCO3- 2.907e-008 2.701e-008 -7.537 -7.569 -0.032

NaHCO3 1.154e-008 1.155e-008 -7.938 -7.938 0.000

Ca 1.167e-003

Ca+2 9.643e-004 7.235e-004 -3.016 -3.141 -0.125

CaCO3 1.685e-004 1.687e-004 -3.773 -3.773 0.000

CaHCO3+ 2.334e-005 2.172e-005 -4.632 -4.663 -0.031

CaSO4 1.099e-005 1.100e-005 -4.959 -4.959 0.000

CaOH+ 1.450e-007 1.347e-007 -6.839 -6.871 -0.032

CaHSO4+ 6.533e-014 6.070e-014 -13.185 -13.217 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.317e-005 -4.242 -4.274 -0.032

H(0) 1.077e-029

H2 5.386e-030 5.392e-030 -29.269 -29.268 0.000

K 3.326e-006

K+ 3.324e-006 3.086e-006 -5.478 -5.511 -0.032

KSO4- 1.840e-009 1.709e-009 -8.735 -8.767 -0.032

KOH 1.199e-011 1.200e-011 -10.921 -10.921 0.000

Mg 5.184e-004

Mg+2 4.557e-004 3.430e-004 -3.341 -3.465 -0.123

MgCO3 4.420e-005 4.424e-005 -4.355 -4.354 0.000

MgHCO3+ 9.780e-006 9.086e-006 -5.010 -5.042 -0.032

MgSO4 6.558e-006 6.565e-006 -5.183 -5.183 0.000

MgOH+ 2.201e-006 2.045e-006 -5.657 -5.689 -0.032

Na 1.001e-005

Na+ 9.963e-006 9.262e-006 -5.002 -5.033 -0.032

NaCO3- 2.907e-008 2.701e-008 -7.537 -7.569 -0.032

NaHCO3 1.154e-008 1.155e-008 -7.938 -7.938 0.000

NaSO4- 3.758e-009 3.492e-009 -8.425 -8.457 -0.032

NaOH 6.858e-011 6.865e-011 -10.164 -10.163 0.000

O(0) 8.040e-004

O2 4.020e-004 4.024e-004 -3.396 -3.395 0.000

S(6) 1.154e-004

SO4-2 9.782e-005 7.324e-005 -4.010 -4.135 -0.126

CaSO4 1.099e-005 1.100e-005 -4.959 -4.959 0.000

MgSO4 6.558e-006 6.565e-006 -5.183 -5.183 0.000

NaSO4- 3.758e-009 3.492e-009 -8.425 -8.457 -0.032

KSO4- 1.840e-009 1.709e-009 -8.735 -8.767 -0.032

HSO4- 7.511e-012 6.978e-012 -11.124 -11.156 -0.032

CaHSO4+ 6.533e-014 6.070e-014 -13.185 -13.217 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.28 -4.38 CaSO4

Aragonite 1.33 -7.04 -8.36 CaCO3

Calcite 1.47 -7.04 -8.51 CaCO3

CO2(g) -3.86 -5.37 -1.52 CO2

Dolomite 2.79 -14.40 -17.19 CaMg(CO3)2

Gypsum -2.69 -7.28 -4.58 CaSO4:2H2O

H2(g) -26.10 -29.27 -3.17 H2

H2O(g) -1.40 -0.00 1.40 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.47 -3.40 -2.92 O2

Initial solution 7. 29/8/2012 13:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.217e-003 3.217e-003

Ca 1.175e-003 1.175e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 8.846e-004 8.846e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.060

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 322

Density (g/cm3) = 0.99597

Activity of water = 1.000

Ionic strength = 4.631e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.808e-003

Total CO2 (mol/kg) = 2.808e-003

Temperature (deg C) = 29.680

Electrical balance (eq) = -1.058e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.80

Iterations = 7

Total H = 1.110149e+002

Total O = 5.551600e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.2399 0.6753

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.749e-005 1.624e-005 -4.757 -4.790 -0.032

H+ 9.313e-010 8.710e-010 -9.031 -9.060 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.808e-003

HCO3- 2.376e-003 2.212e-003 -2.624 -2.655 -0.031

CaCO3 1.749e-004 1.751e-004 -3.757 -3.757 0.000

CO3-2 1.734e-004 1.301e-004 -3.761 -3.886 -0.125

MgCO3 4.556e-005 4.560e-005 -4.341 -4.341 0.000

CaHCO3+ 2.341e-005 2.179e-005 -4.631 -4.662 -0.031

MgHCO3+ 9.743e-006 9.051e-006 -5.011 -5.043 -0.032

CO2 4.110e-006 4.114e-006 -5.386 -5.386 0.000

NaCO3- 3.047e-008 2.831e-008 -7.516 -7.548 -0.032

NaHCO3 1.150e-008 1.152e-008 -7.939 -7.939 0.000

Ca 1.175e-003

Ca+2 9.652e-004 7.239e-004 -3.015 -3.140 -0.125

CaCO3 1.749e-004 1.751e-004 -3.757 -3.757 0.000

CaHCO3+ 2.341e-005 2.179e-005 -4.631 -4.662 -0.031

CaSO4 1.102e-005 1.103e-005 -4.958 -4.957 0.000

CaOH+ 1.485e-007 1.379e-007 -6.828 -6.860 -0.032

CaHSO4+ 6.440e-014 5.983e-014 -13.191 -13.223 -0.032

Cl 5.728e-005

Cl- 5.728e-005 5.317e-005 -4.242 -4.274 -0.032

H(0) 1.025e-029

H2 5.124e-030 5.129e-030 -29.290 -29.290 0.000

K 3.326e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.850e-009 1.719e-009 -8.733 -8.765 -0.032

KOH 1.227e-011 1.228e-011 -10.911 -10.911 0.000

Mg 5.184e-004

Mg+2 4.542e-004 3.418e-004 -3.343 -3.466 -0.124

MgCO3 4.556e-005 4.560e-005 -4.341 -4.341 0.000

MgHCO3+ 9.743e-006 9.051e-006 -5.011 -5.043 -0.032

MgSO4 6.593e-006 6.600e-006 -5.181 -5.180 0.000

MgOH+ 2.325e-006 2.160e-006 -5.634 -5.666 -0.032

Na 1.001e-005

Na+ 9.961e-006 9.260e-006 -5.002 -5.033 -0.032

NaCO3- 3.047e-008 2.831e-008 -7.516 -7.548 -0.032

NaHCO3 1.150e-008 1.152e-008 -7.939 -7.939 0.000

NaSO4- 3.763e-009 3.496e-009 -8.424 -8.456 -0.032

NaOH 7.016e-011 7.024e-011 -10.154 -10.153 0.000

O(0) 8.846e-004

O2 4.423e-004 4.428e-004 -3.354 -3.354 0.000

S(6) 1.154e-004

SO4-2 9.775e-005 7.316e-005 -4.010 -4.136 -0.126

CaSO4 1.102e-005 1.103e-005 -4.958 -4.957 0.000

MgSO4 6.593e-006 6.600e-006 -5.181 -5.180 0.000

NaSO4- 3.763e-009 3.496e-009 -8.424 -8.456 -0.032

KSO4- 1.850e-009 1.719e-009 -8.733 -8.765 -0.032

HSO4- 7.400e-012 6.874e-012 -11.131 -11.163 -0.032

CaHSO4+ 6.440e-014 5.983e-014 -13.191 -13.223 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.28 -4.38 CaSO4

Aragonite 1.34 -7.03 -8.37 CaCO3

Calcite 1.48 -7.03 -8.51 CaCO3

CO2(g) -3.86 -5.39 -1.52 CO2

Dolomite 2.82 -14.38 -17.20 CaMg(CO3)2

Gypsum -2.69 -7.28 -4.58 CaSO4:2H2O

H2(g) -26.12 -29.29 -3.17 H2

H2O(g) -1.39 -0.00 1.39 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.43 -3.35 -2.92 O2

Initial solution 8. 29/8/2012 13:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.207e-003 3.207e-003

Ca 1.171e-003 1.171e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.290e-004 9.290e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.050

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 324

Density (g/cm3) = 0.99585

Activity of water = 1.000

Ionic strength = 4.621e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.802e-003

Total CO2 (mol/kg) = 2.802e-003

Temperature (deg C) = 30.070

Electrical balance (eq) = -1.028e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.75

Iterations = 7

Total H = 1.110149e+002

Total O = 5.551603e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.2239 0.6753

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.758e-005 1.632e-005 -4.755 -4.787 -0.032

H+ 9.530e-010 8.913e-010 -9.021 -9.050 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.802e-003

HCO3- 2.376e-003 2.211e-003 -2.624 -2.655 -0.031

CaCO3 1.733e-004 1.735e-004 -3.761 -3.761 0.000

CO3-2 1.706e-004 1.280e-004 -3.768 -3.893 -0.125

MgCO3 4.512e-005 4.516e-005 -4.346 -4.345 0.000

CaHCO3+ 2.347e-005 2.184e-005 -4.630 -4.661 -0.031

MgHCO3+ 9.768e-006 9.074e-006 -5.010 -5.042 -0.032

CO2 4.188e-006 4.193e-006 -5.378 -5.377 0.000

NaCO3- 3.055e-008 2.838e-008 -7.515 -7.547 -0.032

NaHCO3 1.150e-008 1.151e-008 -7.939 -7.939 0.000

Ca 1.171e-003

Ca+2 9.631e-004 7.224e-004 -3.016 -3.141 -0.125

CaCO3 1.733e-004 1.735e-004 -3.761 -3.761 0.000

CaHCO3+ 2.347e-005 2.184e-005 -4.630 -4.661 -0.031

CaSO4 1.103e-005 1.104e-005 -4.958 -4.957 0.000

CaOH+ 1.448e-007 1.345e-007 -6.839 -6.871 -0.032

CaHSO4+ 6.630e-014 6.159e-014 -13.178 -13.210 -0.032

Cl 5.728e-005

Cl- 5.728e-005 5.317e-005 -4.242 -4.274 -0.032

H(0) 1.069e-029

H2 5.345e-030 5.351e-030 -29.272 -29.272 0.000

K 3.326e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.861e-009 1.729e-009 -8.730 -8.762 -0.032

KOH 1.199e-011 1.200e-011 -10.921 -10.921 0.000

Mg 5.184e-004

Mg+2 4.545e-004 3.420e-004 -3.342 -3.466 -0.123

MgCO3 4.512e-005 4.516e-005 -4.346 -4.345 0.000

MgHCO3+ 9.768e-006 9.074e-006 -5.010 -5.042 -0.032

MgSO4 6.658e-006 6.665e-006 -5.177 -5.176 0.000

MgOH+ 2.352e-006 2.185e-006 -5.628 -5.660 -0.032

Na 1.001e-005

Na+ 9.961e-006 9.260e-006 -5.002 -5.033 -0.032

NaCO3- 3.055e-008 2.838e-008 -7.515 -7.547 -0.032

NaHCO3 1.150e-008 1.151e-008 -7.939 -7.939 0.000

NaSO4- 3.770e-009 3.502e-009 -8.424 -8.456 -0.032

NaOH 6.857e-011 6.864e-011 -10.164 -10.163 0.000

O(0) 9.290e-004

O2 4.645e-004 4.650e-004 -3.333 -3.333 0.000

S(6) 1.154e-004

SO4-2 9.768e-005 7.311e-005 -4.010 -4.136 -0.126

CaSO4 1.103e-005 1.104e-005 -4.958 -4.957 0.000

MgSO4 6.658e-006 6.665e-006 -5.177 -5.176 0.000

NaSO4- 3.770e-009 3.502e-009 -8.424 -8.456 -0.032

KSO4- 1.861e-009 1.729e-009 -8.730 -8.762 -0.032

HSO4- 7.634e-012 7.092e-012 -11.117 -11.149 -0.032

CaHSO4+ 6.630e-014 6.159e-014 -13.178 -13.210 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.28 -4.39 CaSO4

Aragonite 1.34 -7.03 -8.37 CaCO3

Calcite 1.48 -7.03 -8.51 CaCO3

CO2(g) -3.85 -5.38 -1.53 CO2

Dolomite 2.81 -14.39 -17.21 CaMg(CO3)2

Gypsum -2.69 -7.28 -4.58 CaSO4:2H2O

H2(g) -26.10 -29.27 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.41 -3.33 -2.93 O2

Initial solution 9. 29/8/2012 13:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.176e-003 3.176e-003

Ca 1.160e-003 1.160e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.309e-004 9.309e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.030

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 324

Density (g/cm3) = 0.99577

Activity of water = 1.000

Ionic strength = 4.601e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.787e-003

Total CO2 (mol/kg) = 2.787e-003

Temperature (deg C) = 30.330

Electrical balance (eq) = -9.448e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.61

Iterations = 7

Total H = 1.110149e+002

Total O = 5.551599e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.2233 0.6758

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.710e-005 1.588e-005 -4.767 -4.799 -0.032

H+ 9.978e-010 9.333e-010 -9.001 -9.030 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.787e-003

HCO3- 2.376e-003 2.211e-003 -2.624 -2.655 -0.031

CaCO3 1.666e-004 1.667e-004 -3.778 -3.778 0.000

CO3-2 1.636e-004 1.228e-004 -3.786 -3.911 -0.124

MgCO3 4.362e-005 4.366e-005 -4.360 -4.360 0.000

CaHCO3+ 2.344e-005 2.182e-005 -4.630 -4.661 -0.031

MgHCO3+ 9.817e-006 9.121e-006 -5.008 -5.040 -0.032

CO2 4.376e-006 4.380e-006 -5.359 -5.359 0.000

NaCO3- 2.969e-008 2.759e-008 -7.527 -7.559 -0.032

NaHCO3 1.151e-008 1.152e-008 -7.939 -7.939 0.000

Ca 1.160e-003

Ca+2 9.586e-004 7.193e-004 -3.018 -3.143 -0.125

CaCO3 1.666e-004 1.667e-004 -3.778 -3.778 0.000

CaHCO3+ 2.344e-005 2.182e-005 -4.630 -4.661 -0.031

CaSO4 1.101e-005 1.102e-005 -4.958 -4.958 0.000

CaOH+ 1.377e-007 1.279e-007 -6.861 -6.893 -0.032

CaHSO4+ 6.953e-014 6.460e-014 -13.158 -13.190 -0.032

Cl 5.728e-005

Cl- 5.728e-005 5.317e-005 -4.242 -4.274 -0.032

H(0) 1.169e-029

H2 5.846e-030 5.853e-030 -29.233 -29.233 0.000

K 3.326e-006

K+ 3.324e-006 3.086e-006 -5.478 -5.511 -0.032

KSO4- 1.869e-009 1.737e-009 -8.728 -8.760 -0.032

KOH 1.145e-011 1.146e-011 -10.941 -10.941 0.000

Mg 5.184e-004

Mg+2 4.559e-004 3.432e-004 -3.341 -3.464 -0.123

MgCO3 4.362e-005 4.366e-005 -4.360 -4.360 0.000

MgHCO3+ 9.817e-006 9.121e-006 -5.008 -5.040 -0.032

MgSO4 6.725e-006 6.732e-006 -5.172 -5.172 0.000

MgOH+ 2.306e-006 2.143e-006 -5.637 -5.669 -0.032

Na 1.001e-005

Na+ 9.962e-006 9.262e-006 -5.002 -5.033 -0.032

NaCO3- 2.969e-008 2.759e-008 -7.527 -7.559 -0.032

NaHCO3 1.151e-008 1.152e-008 -7.939 -7.939 0.000

NaSO4- 3.776e-009 3.508e-009 -8.423 -8.455 -0.032

NaOH 6.549e-011 6.556e-011 -10.184 -10.183 0.000

O(0) 9.309e-004

O2 4.654e-004 4.659e-004 -3.332 -3.332 0.000

S(6) 1.154e-004

SO4-2 9.764e-005 7.311e-005 -4.010 -4.136 -0.126

CaSO4 1.101e-005 1.102e-005 -4.958 -4.958 0.000

MgSO4 6.725e-006 6.732e-006 -5.172 -5.172 0.000

NaSO4- 3.776e-009 3.508e-009 -8.423 -8.455 -0.032

KSO4- 1.869e-009 1.737e-009 -8.728 -8.760 -0.032

HSO4- 8.040e-012 7.470e-012 -11.095 -11.127 -0.032

CaHSO4+ 6.953e-014 6.460e-014 -13.158 -13.190 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.28 -4.39 CaSO4

Aragonite 1.32 -7.05 -8.37 CaCO3

Calcite 1.46 -7.05 -8.51 CaCO3

CO2(g) -3.83 -5.36 -1.53 CO2

Dolomite 2.78 -14.43 -17.21 CaMg(CO3)2

Gypsum -2.70 -7.28 -4.58 CaSO4:2H2O

H2(g) -26.06 -29.23 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.40 -3.33 -2.93 O2

Initial solution 10. 29/8/2012 14:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.186e-003 3.186e-003

Ca 1.164e-003 1.164e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.290e-004 9.290e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.030

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 327

Density (g/cm3) = 0.99568

Activity of water = 1.000

Ionic strength = 4.606e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.793e-003

Total CO2 (mol/kg) = 2.793e-003

Temperature (deg C) = 30.620

Electrical balance (eq) = -9.732e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.66

Iterations = 7

Total H = 1.110149e+002

Total O = 5.551600e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.1999 0.6750

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.746e-005 1.621e-005 -4.758 -4.790 -0.032

H+ 9.978e-010 9.333e-010 -9.001 -9.030 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.793e-003

HCO3- 2.378e-003 2.213e-003 -2.624 -2.655 -0.031

CaCO3 1.689e-004 1.691e-004 -3.772 -3.772 0.000

CO3-2 1.646e-004 1.236e-004 -3.784 -3.908 -0.125

MgCO3 4.401e-005 4.406e-005 -4.356 -4.356 0.000

CaHCO3+ 2.357e-005 2.194e-005 -4.628 -4.659 -0.031

MgHCO3+ 9.829e-006 9.131e-006 -5.008 -5.039 -0.032

CO2 4.368e-006 4.372e-006 -5.360 -5.359 0.000

NaCO3- 3.029e-008 2.814e-008 -7.519 -7.551 -0.032

NaHCO3 1.151e-008 1.153e-008 -7.939 -7.938 0.000

Ca 1.164e-003

Ca+2 9.599e-004 7.201e-004 -3.018 -3.143 -0.125

CaCO3 1.689e-004 1.691e-004 -3.772 -3.772 0.000

CaHCO3+ 2.357e-005 2.194e-005 -4.628 -4.659 -0.031

CaSO4 1.104e-005 1.105e-005 -4.957 -4.957 0.000

CaOH+ 1.378e-007 1.280e-007 -6.861 -6.893 -0.032

CaHSO4+ 7.000e-014 6.503e-014 -13.155 -13.187 -0.032

Cl 5.728e-005

Cl- 5.728e-005 5.317e-005 -4.242 -4.274 -0.032

H(0) 1.166e-029

H2 5.830e-030 5.836e-030 -29.234 -29.234 0.000

K 3.326e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.877e-009 1.743e-009 -8.727 -8.759 -0.032

KOH 1.145e-011 1.146e-011 -10.941 -10.941 0.000

Mg 5.184e-004

Mg+2 4.554e-004 3.428e-004 -3.342 -3.465 -0.123

MgCO3 4.401e-005 4.406e-005 -4.356 -4.356 0.000

MgHCO3+ 9.829e-006 9.131e-006 -5.008 -5.039 -0.032

MgSO4 6.758e-006 6.765e-006 -5.170 -5.170 0.000

MgOH+ 2.362e-006 2.194e-006 -5.627 -5.659 -0.032

Na 1.001e-005

Na+ 9.962e-006 9.260e-006 -5.002 -5.033 -0.032

NaCO3- 3.029e-008 2.814e-008 -7.519 -7.551 -0.032

NaHCO3 1.151e-008 1.153e-008 -7.939 -7.938 0.000

NaSO4- 3.779e-009 3.510e-009 -8.423 -8.455 -0.032

NaOH 6.548e-011 6.555e-011 -10.184 -10.183 0.000

O(0) 9.290e-004

O2 4.645e-004 4.650e-004 -3.333 -3.333 0.000

S(6) 1.154e-004

SO4-2 9.757e-005 7.304e-005 -4.011 -4.136 -0.126

CaSO4 1.104e-005 1.105e-005 -4.957 -4.957 0.000

MgSO4 6.758e-006 6.765e-006 -5.170 -5.170 0.000

NaSO4- 3.779e-009 3.510e-009 -8.423 -8.455 -0.032

KSO4- 1.877e-009 1.743e-009 -8.727 -8.759 -0.032

HSO4- 8.086e-012 7.512e-012 -11.092 -11.124 -0.032

CaHSO4+ 7.000e-014 6.503e-014 -13.155 -13.187 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.28 -4.39 CaSO4

Aragonite 1.32 -7.05 -8.37 CaCO3

Calcite 1.46 -7.05 -8.51 CaCO3

CO2(g) -3.83 -5.36 -1.53 CO2

Dolomite 2.79 -14.42 -17.22 CaMg(CO3)2

Gypsum -2.69 -7.28 -4.58 CaSO4:2H2O

H2(g) -26.06 -29.23 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.40 -3.33 -2.93 O2

Initial solution 11. 29/8/2012 14:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.186e-003 3.186e-003

Ca 1.164e-003 1.164e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.428e-004 9.428e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.980

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 330

Density (g/cm3) = 0.99564

Activity of water = 1.000

Ionic strength = 4.636e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.825e-003

Total CO2 (mol/kg) = 2.825e-003

Temperature (deg C) = 30.760

Electrical balance (eq) = -9.732e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.65

Iterations = 7

Total H = 1.110149e+002

Total O = 5.551611e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.2403 0.6778

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.572e-005 1.459e-005 -4.803 -4.836 -0.032

H+ 1.120e-009 1.047e-009 -8.951 -8.980 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.825e-003

HCO3- 2.437e-003 2.268e-003 -2.613 -2.644 -0.031

CaCO3 1.568e-004 1.569e-004 -3.805 -3.804 0.000

CO3-2 1.508e-004 1.131e-004 -3.821 -3.946 -0.125

MgCO3 4.063e-005 4.067e-005 -4.391 -4.391 0.000

CaHCO3+ 2.446e-005 2.276e-005 -4.612 -4.643 -0.031

MgHCO3+ 1.014e-005 9.422e-006 -4.994 -5.026 -0.032

CO2 5.015e-006 5.021e-006 -5.300 -5.299 0.000

NaCO3- 2.793e-008 2.594e-008 -7.554 -7.586 -0.032

NaHCO3 1.180e-008 1.181e-008 -7.928 -7.928 0.000

Ca 1.164e-003

Ca+2 9.710e-004 7.278e-004 -3.013 -3.138 -0.125

CaCO3 1.568e-004 1.569e-004 -3.805 -3.804 0.000

CaHCO3+ 2.446e-005 2.276e-005 -4.612 -4.643 -0.031

CaSO4 1.114e-005 1.115e-005 -4.953 -4.953 0.000

CaOH+ 1.242e-007 1.153e-007 -6.906 -6.938 -0.032

CaHSO4+ 7.946e-014 7.380e-014 -13.100 -13.132 -0.032

Cl 5.728e-005

Cl- 5.728e-005 5.316e-005 -4.242 -4.274 -0.032

H(0) 1.466e-029

H2 7.330e-030 7.338e-030 -29.135 -29.134 0.000

K 3.326e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.876e-009 1.743e-009 -8.727 -8.759 -0.032

KOH 1.020e-011 1.021e-011 -10.991 -10.991 0.000

Mg 5.184e-004

Mg+2 4.587e-004 3.449e-004 -3.338 -3.462 -0.124

MgCO3 4.063e-005 4.067e-005 -4.391 -4.391 0.000

MgHCO3+ 1.014e-005 9.422e-006 -4.994 -5.026 -0.032

MgSO4 6.806e-006 6.814e-006 -5.167 -5.167 0.000

MgOH+ 2.145e-006 1.992e-006 -5.669 -5.701 -0.032

Na 1.001e-005

Na+ 9.964e-006 9.260e-006 -5.002 -5.033 -0.032

NaCO3- 2.793e-008 2.594e-008 -7.554 -7.586 -0.032

NaHCO3 1.180e-008 1.181e-008 -7.928 -7.928 0.000

NaSO4- 3.773e-009 3.505e-009 -8.423 -8.455 -0.032

NaOH 5.836e-011 5.842e-011 -10.234 -10.233 0.000

O(0) 9.428e-004

O2 4.714e-004 4.719e-004 -3.327 -3.326 0.000

S(6) 1.154e-004

SO4-2 9.742e-005 7.286e-005 -4.011 -4.138 -0.126

CaSO4 1.114e-005 1.115e-005 -4.953 -4.953 0.000

MgSO4 6.806e-006 6.814e-006 -5.167 -5.167 0.000

NaSO4- 3.773e-009 3.505e-009 -8.423 -8.455 -0.032

KSO4- 1.876e-009 1.743e-009 -8.727 -8.759 -0.032

HSO4- 9.081e-012 8.435e-012 -11.042 -11.074 -0.032

CaHSO4+ 7.946e-014 7.380e-014 -13.100 -13.132 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.28 -4.39 CaSO4

Aragonite 1.29 -7.08 -8.37 CaCO3

Calcite 1.43 -7.08 -8.51 CaCO3

CO2(g) -3.77 -5.30 -1.53 CO2

Dolomite 2.73 -14.49 -17.22 CaMg(CO3)2

Gypsum -2.69 -7.28 -4.58 CaSO4:2H2O

H2(g) -25.96 -29.13 -3.17 H2

H2O(g) -1.36 -0.00 1.36 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.39 -3.33 -2.93 O2

Initial solution 12. 29/8/2012 14:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.155e-003 3.155e-003

Ca 1.152e-003 1.152e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.496e-004 9.496e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.960

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 329

Density (g/cm3) = 0.99559

Activity of water = 1.000

Ionic strength = 4.617e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.810e-003

Total CO2 (mol/kg) = 2.810e-003

Temperature (deg C) = 30.910

Electrical balance (eq) = -8.880e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.51

Iterations = 7

Total H = 1.110149e+002

Total O = 5.551607e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.2492 0.6786

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.518e-005 1.408e-005 -4.819 -4.851 -0.032

H+ 1.172e-009 1.096e-009 -8.931 -8.960 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.810e-003

HCO3- 2.437e-003 2.268e-003 -2.613 -2.644 -0.031

CaCO3 1.500e-004 1.502e-004 -3.824 -3.823 0.000

CO3-2 1.443e-004 1.083e-004 -3.841 -3.965 -0.125

MgCO3 3.913e-005 3.917e-005 -4.408 -4.407 0.000

CaHCO3+ 2.440e-005 2.270e-005 -4.613 -4.644 -0.031

MgHCO3+ 1.019e-005 9.463e-006 -4.992 -5.024 -0.032

CO2 5.243e-006 5.249e-006 -5.280 -5.280 0.000

NaCO3- 2.693e-008 2.502e-008 -7.570 -7.602 -0.032

NaHCO3 1.180e-008 1.181e-008 -7.928 -7.928 0.000

Ca 1.152e-003

Ca+2 9.666e-004 7.248e-004 -3.015 -3.140 -0.125

CaCO3 1.500e-004 1.502e-004 -3.824 -3.823 0.000

CaHCO3+ 2.440e-005 2.270e-005 -4.613 -4.644 -0.031

CaSO4 1.111e-005 1.112e-005 -4.954 -4.954 0.000

CaOH+ 1.181e-007 1.097e-007 -6.928 -6.960 -0.032

CaHSO4+ 8.316e-014 7.725e-014 -13.080 -13.112 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.316e-005 -4.242 -4.274 -0.032

H(0) 1.605e-029

H2 8.026e-030 8.034e-030 -29.096 -29.095 0.000

K 3.326e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.881e-009 1.748e-009 -8.726 -8.758 -0.032

KOH 9.745e-012 9.755e-012 -11.011 -11.011 0.000

Mg 5.184e-004

Mg+2 4.602e-004 3.462e-004 -3.337 -3.461 -0.124

MgCO3 3.913e-005 3.917e-005 -4.408 -4.407 0.000

MgHCO3+ 1.019e-005 9.463e-006 -4.992 -5.024 -0.032

MgSO4 6.858e-006 6.866e-006 -5.164 -5.163 0.000

MgOH+ 2.082e-006 1.934e-006 -5.681 -5.713 -0.032

Na 1.001e-005

Na+ 9.965e-006 9.262e-006 -5.002 -5.033 -0.032

NaCO3- 2.693e-008 2.502e-008 -7.570 -7.602 -0.032

NaHCO3 1.180e-008 1.181e-008 -7.928 -7.928 0.000

NaSO4- 3.778e-009 3.509e-009 -8.423 -8.455 -0.032

NaOH 5.575e-011 5.581e-011 -10.254 -10.253 0.000

O(0) 9.496e-004

O2 4.748e-004 4.753e-004 -3.323 -3.323 0.000

S(6) 1.154e-004

SO4-2 9.739e-005 7.287e-005 -4.011 -4.137 -0.126

CaSO4 1.111e-005 1.112e-005 -4.954 -4.954 0.000

MgSO4 6.858e-006 6.866e-006 -5.164 -5.163 0.000

NaSO4- 3.778e-009 3.509e-009 -8.423 -8.455 -0.032

KSO4- 1.881e-009 1.748e-009 -8.726 -8.758 -0.032

HSO4- 9.543e-012 8.864e-012 -11.020 -11.052 -0.032

CaHSO4+ 8.316e-014 7.725e-014 -13.080 -13.112 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.28 -4.39 CaSO4

Aragonite 1.27 -7.11 -8.38 CaCO3

Calcite 1.41 -7.11 -8.52 CaCO3

CO2(g) -3.75 -5.28 -1.53 CO2

Dolomite 2.69 -14.53 -17.22 CaMg(CO3)2

Gypsum -2.69 -7.28 -4.58 CaSO4:2H2O

H2(g) -25.92 -29.10 -3.18 H2

H2O(g) -1.36 -0.00 1.36 H2O

Halite -10.90 -9.31 1.60 NaCl

O2(g) -0.39 -3.32 -2.93 O2

Initial solution 13. 29/8/2012 14:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.990e-003 2.990e-003

Ca 1.092e-003 1.092e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.709e-004 9.709e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.050

pe = 4.000

Specific Conductance (uS/cm, 31 oC) = 315

Density (g/cm3) = 0.99552

Activity of water = 1.000

Ionic strength = 4.400e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.609e-003

Total CO2 (mol/kg) = 2.609e-003

Temperature (deg C) = 31.120

Electrical balance (eq) = -4.336e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 7

Total H = 1.110147e+002

Total O = 5.551549e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.1449 0.6728

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.892e-005 1.759e-005 -4.723 -4.755 -0.032

H+ 9.518e-010 8.913e-010 -9.021 -9.050 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.609e-003

HCO3- 2.211e-003 2.061e-003 -2.655 -2.686 -0.031

CO3-2 1.610e-004 1.215e-004 -3.793 -3.915 -0.122

CaCO3 1.588e-004 1.590e-004 -3.799 -3.799 0.000

MgCO3 4.388e-005 4.393e-005 -4.358 -4.357 0.000

CaHCO3+ 2.083e-005 1.942e-005 -4.681 -4.712 -0.031

MgHCO3+ 9.220e-006 8.578e-006 -5.035 -5.067 -0.031

CO2 3.866e-006 3.870e-006 -5.413 -5.412 0.000

NaCO3- 3.052e-008 2.839e-008 -7.515 -7.547 -0.031

NaHCO3 1.074e-008 1.075e-008 -7.969 -7.969 0.000

Ca 1.092e-003

Ca+2 9.020e-004 6.804e-004 -3.045 -3.167 -0.122

CaCO3 1.588e-004 1.590e-004 -3.799 -3.799 0.000

CaHCO3+ 2.083e-005 1.942e-005 -4.681 -4.712 -0.031

CaSO4 1.057e-005 1.058e-005 -4.976 -4.976 0.000

CaOH+ 1.362e-007 1.267e-007 -6.866 -6.897 -0.031

CaHSO4+ 6.435e-014 5.987e-014 -13.191 -13.223 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.325e-005 -4.242 -4.274 -0.032

H(0) 1.058e-029

H2 5.292e-030 5.297e-030 -29.276 -29.276 0.000

K 3.326e-006

K+ 3.324e-006 3.090e-006 -5.478 -5.510 -0.032

KSO4- 1.909e-009 1.776e-009 -8.719 -8.751 -0.031

KOH 1.201e-011 1.202e-011 -10.921 -10.920 0.000

Mg 5.184e-004

Mg+2 4.558e-004 3.449e-004 -3.341 -3.462 -0.121

MgCO3 4.388e-005 4.393e-005 -4.358 -4.357 0.000

MgHCO3+ 9.220e-006 8.578e-006 -5.035 -5.067 -0.031

MgSO4 6.943e-006 6.951e-006 -5.158 -5.158 0.000

MgOH+ 2.595e-006 2.414e-006 -5.586 -5.617 -0.031

Na 1.001e-005

Na+ 9.962e-006 9.274e-006 -5.002 -5.033 -0.031

NaCO3- 3.052e-008 2.839e-008 -7.515 -7.547 -0.031

NaHCO3 1.074e-008 1.075e-008 -7.969 -7.969 0.000

NaSO4- 3.823e-009 3.557e-009 -8.418 -8.449 -0.031

NaOH 6.867e-011 6.874e-011 -10.163 -10.163 0.000

O(0) 9.709e-004

O2 4.854e-004 4.859e-004 -3.314 -3.313 0.000

S(6) 1.154e-004

SO4-2 9.785e-005 7.367e-005 -4.009 -4.133 -0.123

CaSO4 1.057e-005 1.058e-005 -4.976 -4.976 0.000

MgSO4 6.943e-006 6.951e-006 -5.158 -5.158 0.000

NaSO4- 3.823e-009 3.557e-009 -8.418 -8.449 -0.031

KSO4- 1.909e-009 1.776e-009 -8.719 -8.751 -0.031

HSO4- 7.866e-012 7.319e-012 -11.104 -11.136 -0.031

CaHSO4+ 6.435e-014 5.987e-014 -13.191 -13.223 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.91 -7.30 -4.39 CaSO4

Aragonite 1.29 -7.08 -8.38 CaCO3

Calcite 1.43 -7.08 -8.52 CaCO3

CO2(g) -3.88 -5.41 -1.54 CO2

Dolomite 2.77 -14.46 -17.23 CaMg(CO3)2

Gypsum -2.72 -7.30 -4.58 CaSO4:2H2O

H2(g) -26.10 -29.28 -3.18 H2

H2O(g) -1.35 -0.00 1.35 H2O

Halite -10.90 -9.31 1.60 NaCl

O2(g) -0.38 -3.31 -2.93 O2

Initial solution 14. 29/8/2012 15:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.990e-003 2.990e-003

Ca 1.092e-003 1.092e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.771e-004 9.771e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.060

pe = 4.000

Specific Conductance (uS/cm, 31 oC) = 315

Density (g/cm3) = 0.99548

Activity of water = 1.000

Ionic strength = 4.392e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.601e-003

Total CO2 (mol/kg) = 2.601e-003

Temperature (deg C) = 31.220

Electrical balance (eq) = -4.336e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 7

Total H = 1.110147e+002

Total O = 5.551548e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.1276 0.6720

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.950e-005 1.813e-005 -4.710 -4.742 -0.032

H+ 9.301e-010 8.710e-010 -9.031 -9.060 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.601e-003

HCO3- 2.197e-003 2.048e-003 -2.658 -2.689 -0.031

CO3-2 1.640e-004 1.238e-004 -3.785 -3.907 -0.122

CaCO3 1.617e-004 1.619e-004 -3.791 -3.791 0.000

MgCO3 4.470e-005 4.474e-005 -4.350 -4.349 0.000

CaHCO3+ 2.067e-005 1.927e-005 -4.685 -4.715 -0.031

MgHCO3+ 9.152e-006 8.516e-006 -5.038 -5.070 -0.031

CO2 3.751e-006 3.755e-006 -5.426 -5.425 0.000

NaCO3- 3.124e-008 2.906e-008 -7.505 -7.537 -0.031

NaHCO3 1.067e-008 1.068e-008 -7.972 -7.971 0.000

Ca 1.092e-003

Ca+2 8.993e-004 6.785e-004 -3.046 -3.168 -0.122

CaCO3 1.617e-004 1.619e-004 -3.791 -3.791 0.000

CaHCO3+ 2.067e-005 1.927e-005 -4.685 -4.715 -0.031

CaSO4 1.055e-005 1.056e-005 -4.977 -4.976 0.000

CaOH+ 1.389e-007 1.293e-007 -6.857 -6.888 -0.031

CaHSO4+ 6.287e-014 5.849e-014 -13.202 -13.233 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.325e-005 -4.242 -4.274 -0.032

H(0) 1.010e-029

H2 5.049e-030 5.054e-030 -29.297 -29.296 0.000

K 3.326e-006

K+ 3.324e-006 3.090e-006 -5.478 -5.510 -0.032

KSO4- 1.912e-009 1.779e-009 -8.718 -8.750 -0.031

KOH 1.229e-011 1.230e-011 -10.911 -10.910 0.000

Mg 5.184e-004

Mg+2 4.549e-004 3.443e-004 -3.342 -3.463 -0.121

MgCO3 4.470e-005 4.474e-005 -4.350 -4.349 0.000

MgHCO3+ 9.152e-006 8.516e-006 -5.038 -5.070 -0.031

MgSO4 6.951e-006 6.958e-006 -5.158 -5.158 0.000

MgOH+ 2.674e-006 2.488e-006 -5.573 -5.604 -0.031

Na 1.001e-005

Na+ 9.961e-006 9.274e-006 -5.002 -5.033 -0.031

NaCO3- 3.124e-008 2.906e-008 -7.505 -7.537 -0.031

NaHCO3 1.067e-008 1.068e-008 -7.972 -7.971 0.000

NaSO4- 3.826e-009 3.560e-009 -8.417 -8.449 -0.031

NaOH 7.027e-011 7.034e-011 -10.153 -10.153 0.000

O(0) 9.771e-004

O2 4.886e-004 4.891e-004 -3.311 -3.311 0.000

S(6) 1.154e-004

SO4-2 9.786e-005 7.369e-005 -4.009 -4.133 -0.123

CaSO4 1.055e-005 1.056e-005 -4.977 -4.976 0.000

MgSO4 6.951e-006 6.958e-006 -5.158 -5.158 0.000

NaSO4- 3.826e-009 3.560e-009 -8.417 -8.449 -0.031

KSO4- 1.912e-009 1.779e-009 -8.718 -8.750 -0.031

HSO4- 7.707e-012 7.171e-012 -11.113 -11.144 -0.031

CaHSO4+ 6.287e-014 5.849e-014 -13.202 -13.233 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.91 -7.30 -4.39 CaSO4

Aragonite 1.30 -7.08 -8.38 CaCO3

Calcite 1.44 -7.08 -8.52 CaCO3

CO2(g) -3.89 -5.43 -1.54 CO2

Dolomite 2.79 -14.45 -17.23 CaMg(CO3)2

Gypsum -2.72 -7.30 -4.58 CaSO4:2H2O

H2(g) -26.12 -29.30 -3.18 H2

H2O(g) -1.35 -0.00 1.35 H2O

Halite -10.90 -9.31 1.60 NaCl

O2(g) -0.38 -3.31 -2.93 O2

Initial solution 15. 29/8/2012 15:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.990e-003 2.990e-003

Ca 1.092e-003 1.092e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.940e-004 9.940e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.060

pe = 4.000

Specific Conductance (uS/cm, 31 oC) = 315

Density (g/cm3) = 0.99548

Activity of water = 1.000

Ionic strength = 4.392e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.601e-003

Total CO2 (mol/kg) = 2.601e-003

Temperature (deg C) = 31.220

Electrical balance (eq) = -4.336e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 7

Total H = 1.110147e+002

Total O = 5.551549e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.1295 0.6721

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.950e-005 1.813e-005 -4.710 -4.742 -0.032

H+ 9.301e-010 8.710e-010 -9.031 -9.060 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.601e-003

HCO3- 2.197e-003 2.048e-003 -2.658 -2.689 -0.031

CO3-2 1.640e-004 1.238e-004 -3.785 -3.907 -0.122

CaCO3 1.617e-004 1.619e-004 -3.791 -3.791 0.000

MgCO3 4.470e-005 4.474e-005 -4.350 -4.349 0.000

CaHCO3+ 2.067e-005 1.927e-005 -4.685 -4.715 -0.031

MgHCO3+ 9.152e-006 8.516e-006 -5.038 -5.070 -0.031

CO2 3.751e-006 3.755e-006 -5.426 -5.425 0.000

NaCO3- 3.124e-008 2.906e-008 -7.505 -7.537 -0.031

NaHCO3 1.067e-008 1.068e-008 -7.972 -7.971 0.000

Ca 1.092e-003

Ca+2 8.993e-004 6.785e-004 -3.046 -3.168 -0.122

CaCO3 1.617e-004 1.619e-004 -3.791 -3.791 0.000

CaHCO3+ 2.067e-005 1.927e-005 -4.685 -4.715 -0.031

CaSO4 1.055e-005 1.056e-005 -4.977 -4.976 0.000

CaOH+ 1.389e-007 1.293e-007 -6.857 -6.888 -0.031

CaHSO4+ 6.287e-014 5.849e-014 -13.202 -13.233 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.325e-005 -4.242 -4.274 -0.032

H(0) 1.010e-029

H2 5.049e-030 5.054e-030 -29.297 -29.296 0.000

K 3.326e-006

K+ 3.324e-006 3.090e-006 -5.478 -5.510 -0.032

KSO4- 1.912e-009 1.779e-009 -8.718 -8.750 -0.031

KOH 1.229e-011 1.230e-011 -10.911 -10.910 0.000

Mg 5.184e-004

Mg+2 4.549e-004 3.443e-004 -3.342 -3.463 -0.121

MgCO3 4.470e-005 4.474e-005 -4.350 -4.349 0.000

MgHCO3+ 9.152e-006 8.516e-006 -5.038 -5.070 -0.031

MgSO4 6.951e-006 6.958e-006 -5.158 -5.158 0.000

MgOH+ 2.674e-006 2.488e-006 -5.573 -5.604 -0.031

Na 1.001e-005

Na+ 9.961e-006 9.274e-006 -5.002 -5.033 -0.031

NaCO3- 3.124e-008 2.906e-008 -7.505 -7.537 -0.031

NaHCO3 1.067e-008 1.068e-008 -7.972 -7.971 0.000

NaSO4- 3.826e-009 3.560e-009 -8.417 -8.449 -0.031

NaOH 7.027e-011 7.034e-011 -10.153 -10.153 0.000

O(0) 9.940e-004

O2 4.970e-004 4.975e-004 -3.304 -3.303 0.000

S(6) 1.154e-004

SO4-2 9.786e-005 7.369e-005 -4.009 -4.133 -0.123

CaSO4 1.055e-005 1.056e-005 -4.977 -4.976 0.000

MgSO4 6.951e-006 6.958e-006 -5.158 -5.158 0.000

NaSO4- 3.826e-009 3.560e-009 -8.417 -8.449 -0.031

KSO4- 1.912e-009 1.779e-009 -8.718 -8.750 -0.031

HSO4- 7.707e-012 7.171e-012 -11.113 -11.144 -0.031

CaHSO4+ 6.287e-014 5.849e-014 -13.202 -13.233 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.91 -7.30 -4.39 CaSO4

Aragonite 1.30 -7.08 -8.38 CaCO3

Calcite 1.44 -7.08 -8.52 CaCO3

CO2(g) -3.89 -5.43 -1.54 CO2

Dolomite 2.79 -14.45 -17.23 CaMg(CO3)2

Gypsum -2.72 -7.30 -4.58 CaSO4:2H2O

H2(g) -26.12 -29.30 -3.18 H2

H2O(g) -1.35 -0.00 1.35 H2O

Halite -10.90 -9.31 1.60 NaCl

O2(g) -0.37 -3.30 -2.93 O2

Initial solution 16. 29/8/2012 15:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.953e-004 9.953e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.060

pe = 4.000

Specific Conductance (uS/cm, 31 oC) = 313

Density (g/cm3) = 0.99550

Activity of water = 1.000

Ionic strength = 4.364e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.575e-003

Total CO2 (mol/kg) = 2.575e-003

Temperature (deg C) = 31.170

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.63

Iterations = 7

Total H = 1.110147e+002

Total O = 5.551542e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.1336 0.6722

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.942e-005 1.806e-005 -4.712 -4.743 -0.032

H+ 9.299e-010 8.710e-010 -9.032 -9.060 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.575e-003

HCO3- 2.177e-003 2.030e-003 -2.662 -2.693 -0.030

CO3-2 1.622e-004 1.226e-004 -3.790 -3.912 -0.122

CaCO3 1.587e-004 1.589e-004 -3.799 -3.799 0.000

MgCO3 4.431e-005 4.435e-005 -4.354 -4.353 0.000

CaHCO3+ 2.031e-005 1.893e-005 -4.692 -4.723 -0.030

MgHCO3+ 9.082e-006 8.452e-006 -5.042 -5.073 -0.031

CO2 3.719e-006 3.723e-006 -5.430 -5.429 0.000

NaCO3- 3.086e-008 2.872e-008 -7.511 -7.542 -0.031

NaHCO3 1.058e-008 1.059e-008 -7.976 -7.975 0.000

Ca 1.081e-003

Ca+2 8.915e-004 6.732e-004 -3.050 -3.172 -0.122

CaCO3 1.587e-004 1.589e-004 -3.799 -3.799 0.000

CaHCO3+ 2.031e-005 1.893e-005 -4.692 -4.723 -0.030

CaSO4 1.048e-005 1.049e-005 -4.980 -4.979 0.000

CaOH+ 1.378e-007 1.283e-007 -6.861 -6.892 -0.031

CaHSO4+ 6.238e-014 5.805e-014 -13.205 -13.236 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.326e-005 -4.242 -4.274 -0.032

H(0) 1.010e-029

H2 5.052e-030 5.057e-030 -29.297 -29.296 0.000

K 3.326e-006

K+ 3.324e-006 3.091e-006 -5.478 -5.510 -0.032

KSO4- 1.914e-009 1.781e-009 -8.718 -8.749 -0.031

KOH 1.229e-011 1.230e-011 -10.910 -10.910 0.000

Mg 5.184e-004

Mg+2 4.554e-004 3.449e-004 -3.342 -3.462 -0.121

MgCO3 4.431e-005 4.435e-005 -4.354 -4.353 0.000

MgHCO3+ 9.082e-006 8.452e-006 -5.042 -5.073 -0.031

MgSO4 6.965e-006 6.972e-006 -5.157 -5.157 0.000

MgOH+ 2.667e-006 2.482e-006 -5.574 -5.605 -0.031

Na 1.001e-005

Na+ 9.962e-006 9.276e-006 -5.002 -5.033 -0.031

NaCO3- 3.086e-008 2.872e-008 -7.511 -7.542 -0.031

NaHCO3 1.058e-008 1.059e-008 -7.976 -7.975 0.000

NaSO4- 3.831e-009 3.565e-009 -8.417 -8.448 -0.031

NaOH 7.029e-011 7.036e-011 -10.153 -10.153 0.000

O(0) 9.953e-004

O2 4.976e-004 4.981e-004 -3.303 -3.303 0.000

S(6) 1.154e-004

SO4-2 9.792e-005 7.379e-005 -4.009 -4.132 -0.123

CaSO4 1.048e-005 1.049e-005 -4.980 -4.979 0.000

MgSO4 6.965e-006 6.972e-006 -5.157 -5.157 0.000

NaSO4- 3.831e-009 3.565e-009 -8.417 -8.448 -0.031

KSO4- 1.914e-009 1.781e-009 -8.718 -8.749 -0.031

HSO4- 7.707e-012 7.173e-012 -11.113 -11.144 -0.031

CaHSO4+ 6.238e-014 5.805e-014 -13.205 -13.236 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.91 -7.30 -4.39 CaSO4

Aragonite 1.29 -7.08 -8.38 CaCO3

Calcite 1.43 -7.08 -8.52 CaCO3

CO2(g) -3.89 -5.43 -1.54 CO2

Dolomite 2.77 -14.46 -17.23 CaMg(CO3)2

Gypsum -2.72 -7.30 -4.58 CaSO4:2H2O

H2(g) -26.12 -29.30 -3.18 H2

H2O(g) -1.35 -0.00 1.35 H2O

Halite -10.90 -9.31 1.60 NaCl

O2(g) -0.37 -3.30 -2.93 O2

Initial solution 17. 29/8/2012 15:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.938e-003 2.938e-003

Ca 1.074e-003 1.074e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.953e-004 9.953e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.060

pe = 4.000

Specific Conductance (uS/cm, 31 oC) = 311

Density (g/cm3) = 0.99553

Activity of water = 1.000

Ionic strength = 4.346e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.559e-003

Total CO2 (mol/kg) = 2.559e-003

Temperature (deg C) = 31.070

Electrical balance (eq) = -2.899e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.53

Iterations = 7

Total H = 1.110146e+002

Total O = 5.551537e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.1415 0.6725

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.928e-005 1.793e-005 -4.715 -4.746 -0.032

H+ 9.298e-010 8.710e-010 -9.032 -9.060 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.559e-003

HCO3- 2.165e-003 2.018e-003 -2.665 -2.695 -0.030

CO3-2 1.609e-004 1.217e-004 -3.793 -3.915 -0.121

CaCO3 1.564e-004 1.565e-004 -3.806 -3.805 0.000

MgCO3 4.398e-005 4.402e-005 -4.357 -4.356 0.000

CaHCO3+ 2.007e-005 1.871e-005 -4.698 -4.728 -0.030

MgHCO3+ 9.038e-006 8.412e-006 -5.044 -5.075 -0.031

CO2 3.702e-006 3.706e-006 -5.432 -5.431 0.000

NaCO3- 3.049e-008 2.837e-008 -7.516 -7.547 -0.031

NaHCO3 1.052e-008 1.053e-008 -7.978 -7.978 0.000

Ca 1.074e-003

Ca+2 8.866e-004 6.699e-004 -3.052 -3.174 -0.122

CaCO3 1.564e-004 1.565e-004 -3.806 -3.805 0.000

CaHCO3+ 2.007e-005 1.871e-005 -4.698 -4.728 -0.030

CaSO4 1.043e-005 1.044e-005 -4.982 -4.981 0.000

CaOH+ 1.371e-007 1.276e-007 -6.863 -6.894 -0.031

CaHSO4+ 6.199e-014 5.770e-014 -13.208 -13.239 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.327e-005 -4.242 -4.274 -0.031

H(0) 1.011e-029

H2 5.056e-030 5.061e-030 -29.296 -29.296 0.000

K 3.326e-006

K+ 3.324e-006 3.091e-006 -5.478 -5.510 -0.031

KSO4- 1.912e-009 1.780e-009 -8.718 -8.750 -0.031

KOH 1.229e-011 1.231e-011 -10.910 -10.910 0.000

Mg 5.184e-004

Mg+2 4.558e-004 3.454e-004 -3.341 -3.462 -0.120

MgCO3 4.398e-005 4.402e-005 -4.357 -4.356 0.000

MgHCO3+ 9.038e-006 8.412e-006 -5.044 -5.075 -0.031

MgSO4 6.965e-006 6.972e-006 -5.157 -5.157 0.000

MgOH+ 2.647e-006 2.464e-006 -5.577 -5.608 -0.031

Na 1.001e-005

Na+ 9.962e-006 9.278e-006 -5.002 -5.033 -0.031

NaCO3- 3.049e-008 2.837e-008 -7.516 -7.547 -0.031

NaHCO3 1.052e-008 1.053e-008 -7.978 -7.978 0.000

NaSO4- 3.832e-009 3.567e-009 -8.417 -8.448 -0.031

NaOH 7.031e-011 7.038e-011 -10.153 -10.153 0.000

O(0) 9.953e-004

O2 4.976e-004 4.981e-004 -3.303 -3.303 0.000

S(6) 1.154e-004

SO4-2 9.797e-005 7.387e-005 -4.009 -4.132 -0.123

CaSO4 1.043e-005 1.044e-005 -4.982 -4.981 0.000

MgSO4 6.965e-006 6.972e-006 -5.157 -5.157 0.000

NaSO4- 3.832e-009 3.567e-009 -8.417 -8.448 -0.031

KSO4- 1.912e-009 1.780e-009 -8.718 -8.750 -0.031

HSO4- 7.697e-012 7.164e-012 -11.114 -11.145 -0.031

CaHSO4+ 6.199e-014 5.770e-014 -13.208 -13.239 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.91 -7.31 -4.39 CaSO4

Aragonite 1.29 -7.09 -8.38 CaCO3

Calcite 1.43 -7.09 -8.52 CaCO3

CO2(g) -3.90 -5.43 -1.54 CO2

Dolomite 2.76 -14.47 -17.23 CaMg(CO3)2

Gypsum -2.72 -7.31 -4.58 CaSO4:2H2O

H2(g) -26.12 -29.30 -3.18 H2

H2O(g) -1.36 -0.00 1.36 H2O

Halite -10.90 -9.31 1.60 NaCl

O2(g) -0.37 -3.30 -2.93 O2

Initial solution 18. 29/8/2012 16:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.907e-003 2.907e-003

Ca 1.062e-003 1.062e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.959e-004 9.959e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.050

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 308

Density (g/cm3) = 0.99559

Activity of water = 1.000

Ionic strength = 4.326e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.541e-003

Total CO2 (mol/kg) = 2.541e-003

Temperature (deg C) = 30.870

Electrical balance (eq) = -2.047e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.37

Iterations = 7

Total H = 1.110146e+002

Total O = 5.551531e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.1675 0.6736

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.858e-005 1.728e-005 -4.731 -4.763 -0.031

H+ 9.513e-010 8.913e-010 -9.022 -9.050 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.541e-003

HCO3- 2.158e-003 2.013e-003 -2.666 -2.696 -0.030

CO3-2 1.562e-004 1.182e-004 -3.806 -3.927 -0.121

CaCO3 1.504e-004 1.506e-004 -3.823 -3.822 0.000

MgCO3 4.274e-005 4.278e-005 -4.369 -4.369 0.000

CaHCO3+ 1.986e-005 1.853e-005 -4.702 -4.732 -0.030

MgHCO3+ 9.034e-006 8.410e-006 -5.044 -5.075 -0.031

CO2 3.785e-006 3.789e-006 -5.422 -5.422 0.000

NaCO3- 2.933e-008 2.730e-008 -7.533 -7.564 -0.031

NaHCO3 1.050e-008 1.051e-008 -7.979 -7.979 0.000

Ca 1.062e-003

Ca+2 8.816e-004 6.666e-004 -3.055 -3.176 -0.121

CaCO3 1.504e-004 1.506e-004 -3.823 -3.822 0.000

CaHCO3+ 1.986e-005 1.853e-005 -4.702 -4.732 -0.030

CaSO4 1.037e-005 1.038e-005 -4.984 -4.984 0.000

CaOH+ 1.333e-007 1.241e-007 -6.875 -6.906 -0.031

CaHSO4+ 6.290e-014 5.856e-014 -13.201 -13.232 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.328e-005 -4.242 -4.273 -0.031

H(0) 1.061e-029

H2 5.305e-030 5.310e-030 -29.275 -29.275 0.000

K 3.326e-006

K+ 3.324e-006 3.092e-006 -5.478 -5.510 -0.031

KSO4- 1.908e-009 1.777e-009 -8.719 -8.750 -0.031

KOH 1.202e-011 1.203e-011 -10.920 -10.920 0.000

Mg 5.184e-004

Mg+2 4.571e-004 3.467e-004 -3.340 -3.460 -0.120

MgCO3 4.274e-005 4.278e-005 -4.369 -4.369 0.000

MgHCO3+ 9.034e-006 8.410e-006 -5.044 -5.075 -0.031

MgSO4 6.965e-006 6.972e-006 -5.157 -5.157 0.000

MgOH+ 2.551e-006 2.375e-006 -5.593 -5.624 -0.031

Na 1.001e-005

Na+ 9.963e-006 9.281e-006 -5.002 -5.032 -0.031

NaCO3- 2.933e-008 2.730e-008 -7.533 -7.564 -0.031

NaHCO3 1.050e-008 1.051e-008 -7.979 -7.979 0.000

NaSO4- 3.833e-009 3.568e-009 -8.416 -8.448 -0.031

NaOH 6.873e-011 6.879e-011 -10.163 -10.162 0.000

O(0) 9.959e-004

O2 4.979e-004 4.984e-004 -3.303 -3.302 0.000

S(6) 1.154e-004

SO4-2 9.803e-005 7.397e-005 -4.009 -4.131 -0.122

CaSO4 1.037e-005 1.038e-005 -4.984 -4.984 0.000

MgSO4 6.965e-006 6.972e-006 -5.157 -5.157 0.000

NaSO4- 3.833e-009 3.568e-009 -8.416 -8.448 -0.031

KSO4- 1.908e-009 1.777e-009 -8.719 -8.750 -0.031

HSO4- 7.849e-012 7.307e-012 -11.105 -11.136 -0.031

CaHSO4+ 6.290e-014 5.856e-014 -13.201 -13.232 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.92 -7.31 -4.39 CaSO4

Aragonite 1.27 -7.10 -8.38 CaCO3

Calcite 1.41 -7.10 -8.52 CaCO3

CO2(g) -3.89 -5.42 -1.53 CO2

Dolomite 2.73 -14.49 -17.22 CaMg(CO3)2

Gypsum -2.72 -7.31 -4.58 CaSO4:2H2O

H2(g) -26.10 -29.27 -3.17 H2

H2O(g) -1.36 -0.00 1.36 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.37 -3.30 -2.93 O2

Initial solution 19. 29/8/2012 16:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.866e-003 2.866e-003

Ca 1.047e-003 1.047e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.010e-003 1.010e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.100

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 303

Density (g/cm3) = 0.99562

Activity of water = 1.000

Ionic strength = 4.259e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.474e-003

Total CO2 (mol/kg) = 2.474e-003

Temperature (deg C) = 30.760

Electrical balance (eq) = -9.271e-006

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.17

Iterations = 7

Total H = 1.110146e+002

Total O = 5.551513e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.1278 0.6710

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.067e-005 1.923e-005 -4.685 -4.716 -0.031

H+ 8.475e-010 7.943e-010 -9.072 -9.100 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.474e-003

HCO3- 2.073e-003 1.934e-003 -2.683 -2.714 -0.030

CO3-2 1.677e-004 1.271e-004 -3.775 -3.896 -0.120

CaCO3 1.579e-004 1.580e-004 -3.802 -3.801 0.000

MgCO3 4.571e-005 4.576e-005 -4.340 -4.340 0.000

CaHCO3+ 1.863e-005 1.739e-005 -4.730 -4.760 -0.030

MgHCO3+ 8.633e-006 8.041e-006 -5.064 -5.095 -0.031

CO2 3.244e-006 3.247e-006 -5.489 -5.488 0.000

NaCO3- 3.138e-008 2.923e-008 -7.503 -7.534 -0.031

NaHCO3 1.009e-008 1.010e-008 -7.996 -7.996 0.000

Ca 1.047e-003

Ca+2 8.606e-004 6.520e-004 -3.065 -3.186 -0.121

CaCO3 1.579e-004 1.580e-004 -3.802 -3.801 0.000

CaHCO3+ 1.863e-005 1.739e-005 -4.730 -4.760 -0.030

CaSO4 1.018e-005 1.019e-005 -4.992 -4.992 0.000

CaOH+ 1.462e-007 1.362e-007 -6.835 -6.866 -0.031

CaHSO4+ 5.490e-014 5.113e-014 -13.260 -13.291 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.331e-005 -4.242 -4.273 -0.031

H(0) 8.437e-030

H2 4.218e-030 4.222e-030 -29.375 -29.374 0.000

K 3.325e-006

K+ 3.324e-006 3.093e-006 -5.478 -5.510 -0.031

KSO4- 1.913e-009 1.782e-009 -8.718 -8.749 -0.031

KOH 1.349e-011 1.350e-011 -10.870 -10.870 0.000

Mg 5.184e-004

Mg+2 4.543e-004 3.452e-004 -3.343 -3.462 -0.119

MgCO3 4.571e-005 4.576e-005 -4.340 -4.340 0.000

MgHCO3+ 8.633e-006 8.041e-006 -5.064 -5.095 -0.031

MgSO4 6.946e-006 6.953e-006 -5.158 -5.158 0.000

MgOH+ 2.822e-006 2.628e-006 -5.549 -5.580 -0.031

Na 1.001e-005

Na+ 9.962e-006 9.284e-006 -5.002 -5.032 -0.031

NaCO3- 3.138e-008 2.923e-008 -7.503 -7.534 -0.031

NaHCO3 1.009e-008 1.010e-008 -7.996 -7.996 0.000

NaSO4- 3.846e-009 3.582e-009 -8.415 -8.446 -0.031

NaOH 7.714e-011 7.721e-011 -10.113 -10.112 0.000

O(0) 1.010e-003

O2 5.048e-004 5.053e-004 -3.297 -3.296 0.000

S(6) 1.154e-004

SO4-2 9.824e-005 7.428e-005 -4.008 -4.129 -0.121

CaSO4 1.018e-005 1.019e-005 -4.992 -4.992 0.000

MgSO4 6.946e-006 6.953e-006 -5.158 -5.158 0.000

NaSO4- 3.846e-009 3.582e-009 -8.415 -8.446 -0.031

KSO4- 1.913e-009 1.782e-009 -8.718 -8.749 -0.031

HSO4- 7.004e-012 6.523e-012 -11.155 -11.186 -0.031

CaHSO4+ 5.490e-014 5.113e-014 -13.260 -13.291 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.92 -7.31 -4.39 CaSO4

Aragonite 1.29 -7.08 -8.37 CaCO3

Calcite 1.43 -7.08 -8.51 CaCO3

CO2(g) -3.96 -5.49 -1.53 CO2

Dolomite 2.78 -14.44 -17.22 CaMg(CO3)2

Gypsum -2.73 -7.31 -4.58 CaSO4:2H2O

H2(g) -26.20 -29.37 -3.17 H2

H2O(g) -1.36 -0.00 1.36 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.36 -3.30 -2.93 O2

Initial solution 20. 29/8/2012 16:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.814e-003 2.814e-003

Ca 1.029e-003 1.029e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.004e-003 1.004e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.140

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 297

Density (g/cm3) = 0.99567

Activity of water = 1.000

Ionic strength = 4.190e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.406e-003

Total CO2 (mol/kg) = 2.406e-003

Temperature (deg C) = 30.590

Electrical balance (eq) = 5.094e-006

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.10

Iterations = 7

Total H = 1.110145e+002

Total O = 5.551492e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.1007 0.6690

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.238e-005 2.084e-005 -4.650 -4.681 -0.031

H+ 7.726e-010 7.244e-010 -9.112 -9.140 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.406e-003

HCO3- 1.992e-003 1.860e-003 -2.701 -2.731 -0.030

CO3-2 1.760e-004 1.337e-004 -3.755 -3.874 -0.119

CaCO3 1.616e-004 1.618e-004 -3.791 -3.791 0.000

MgCO3 4.783e-005 4.787e-005 -4.320 -4.320 0.000

CaHCO3+ 1.747e-005 1.631e-005 -4.758 -4.788 -0.030

MgHCO3+ 8.271e-006 7.708e-006 -5.082 -5.113 -0.031

CO2 2.850e-006 2.853e-006 -5.545 -5.545 0.000

NaCO3- 3.272e-008 3.049e-008 -7.485 -7.516 -0.031

NaHCO3 9.705e-009 9.714e-009 -8.013 -8.013 0.000

Ca 1.029e-003

Ca+2 8.395e-004 6.373e-004 -3.076 -3.196 -0.120

CaCO3 1.616e-004 1.618e-004 -3.791 -3.791 0.000

CaHCO3+ 1.747e-005 1.631e-005 -4.758 -4.788 -0.030

CaSO4 9.976e-006 9.985e-006 -5.001 -5.001 0.000

CaOH+ 1.567e-007 1.460e-007 -6.805 -6.836 -0.031

CaHSO4+ 4.894e-014 4.561e-014 -13.310 -13.341 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.334e-005 -4.242 -4.273 -0.031

H(0) 7.029e-030

H2 3.514e-030 3.518e-030 -29.454 -29.454 0.000

K 3.325e-006

K+ 3.324e-006 3.095e-006 -5.478 -5.509 -0.031

KSO4- 1.916e-009 1.785e-009 -8.718 -8.748 -0.031

KOH 1.480e-011 1.481e-011 -10.830 -10.829 0.000

Mg 5.184e-004

Mg+2 4.523e-004 3.444e-004 -3.345 -3.463 -0.118

MgCO3 4.783e-005 4.787e-005 -4.320 -4.320 0.000

MgHCO3+ 8.271e-006 7.708e-006 -5.082 -5.113 -0.031

MgSO4 6.931e-006 6.938e-006 -5.159 -5.159 0.000

MgOH+ 3.040e-006 2.833e-006 -5.517 -5.548 -0.031

Na 1.001e-005

Na+ 9.961e-006 9.288e-006 -5.002 -5.032 -0.030

NaCO3- 3.272e-008 3.049e-008 -7.485 -7.516 -0.031

NaHCO3 9.705e-009 9.714e-009 -8.013 -8.013 0.000

NaSO4- 3.858e-009 3.596e-009 -8.414 -8.444 -0.031

NaOH 8.462e-011 8.470e-011 -10.073 -10.072 0.000

O(0) 1.004e-003

O2 5.020e-004 5.025e-004 -3.299 -3.299 0.000

S(6) 1.154e-004

SO4-2 9.846e-005 7.460e-005 -4.007 -4.127 -0.121

CaSO4 9.976e-006 9.985e-006 -5.001 -5.001 0.000

MgSO4 6.931e-006 6.938e-006 -5.159 -5.159 0.000

NaSO4- 3.858e-009 3.596e-009 -8.414 -8.444 -0.031

KSO4- 1.916e-009 1.785e-009 -8.718 -8.748 -0.031

HSO4- 6.387e-012 5.952e-012 -11.195 -11.225 -0.031

CaHSO4+ 4.894e-014 4.561e-014 -13.310 -13.341 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.93 -7.32 -4.39 CaSO4

Aragonite 1.30 -7.07 -8.37 CaCO3

Calcite 1.44 -7.07 -8.51 CaCO3

CO2(g) -4.01 -5.54 -1.53 CO2

Dolomite 2.81 -14.41 -17.22 CaMg(CO3)2

Gypsum -2.74 -7.32 -4.58 CaSO4:2H2O

H2(g) -26.28 -29.45 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.37 -3.30 -2.93 O2

Initial solution 21. 29/8/2012 16:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.773e-003 2.773e-003

Ca 1.014e-003 1.014e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.004e-003 1.004e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.200

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 291

Density (g/cm3) = 0.99569

Activity of water = 1.000

Ionic strength = 4.117e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.332e-003

Total CO2 (mol/kg) = 2.332e-003

Temperature (deg C) = 30.530

Electrical balance (eq) = 1.646e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.32

Iterations = 7

Total H = 1.110144e+002

Total O = 5.551470e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.0455 0.6655

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.557e-005 2.382e-005 -4.592 -4.623 -0.031

H+ 6.726e-010 6.310e-010 -9.172 -9.200 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.332e-003

HCO3- 1.891e-003 1.766e-003 -2.723 -2.753 -0.030

CO3-2 1.913e-004 1.456e-004 -3.718 -3.837 -0.118

CaCO3 1.713e-004 1.715e-004 -3.766 -3.766 0.000

MgCO3 5.173e-005 5.178e-005 -4.286 -4.286 0.000

CaHCO3+ 1.615e-005 1.509e-005 -4.792 -4.821 -0.030

MgHCO3+ 7.799e-006 7.272e-006 -5.108 -5.138 -0.030

CO2 2.359e-006 2.361e-006 -5.627 -5.627 0.000

NaCO3- 3.553e-008 3.313e-008 -7.449 -7.480 -0.030

NaHCO3 9.221e-009 9.229e-009 -8.035 -8.035 0.000

Ca 1.014e-003

Ca+2 8.163e-004 6.211e-004 -3.088 -3.207 -0.119

CaCO3 1.713e-004 1.715e-004 -3.766 -3.766 0.000

CaHCO3+ 1.615e-005 1.509e-005 -4.792 -4.821 -0.030

CaSO4 9.761e-006 9.770e-006 -5.010 -5.010 0.000

CaOH+ 1.752e-007 1.633e-007 -6.757 -6.787 -0.030

CaHSO4+ 4.165e-014 3.883e-014 -13.380 -13.411 -0.030

Cl 5.727e-005

Cl- 5.727e-005 5.337e-005 -4.242 -4.273 -0.031

H(0) 5.335e-030

H2 2.668e-030 2.670e-030 -29.574 -29.573 0.000

K 3.325e-006

K+ 3.324e-006 3.097e-006 -5.478 -5.509 -0.031

KSO4- 1.923e-009 1.793e-009 -8.716 -8.746 -0.030

KOH 1.700e-011 1.702e-011 -10.770 -10.769 0.000

Mg 5.184e-004

Mg+2 4.485e-004 3.423e-004 -3.348 -3.466 -0.117

MgCO3 5.173e-005 5.178e-005 -4.286 -4.286 0.000

MgHCO3+ 7.799e-006 7.272e-006 -5.108 -5.138 -0.030

MgSO4 6.909e-006 6.915e-006 -5.161 -5.160 0.000

MgOH+ 3.448e-006 3.215e-006 -5.462 -5.493 -0.030

Na 1.001e-005

Na+ 9.958e-006 9.291e-006 -5.002 -5.032 -0.030

NaCO3- 3.553e-008 3.313e-008 -7.449 -7.480 -0.030

NaHCO3 9.221e-009 9.229e-009 -8.035 -8.035 0.000

NaSO4- 3.874e-009 3.612e-009 -8.412 -8.442 -0.030

NaOH 9.719e-011 9.728e-011 -10.012 -10.012 0.000

O(0) 1.004e-003

O2 5.020e-004 5.025e-004 -3.299 -3.299 0.000

S(6) 1.154e-004

SO4-2 9.869e-005 7.494e-005 -4.006 -4.125 -0.120

CaSO4 9.761e-006 9.770e-006 -5.010 -5.010 0.000

MgSO4 6.909e-006 6.915e-006 -5.161 -5.160 0.000

NaSO4- 3.874e-009 3.612e-009 -8.412 -8.442 -0.030

KSO4- 1.923e-009 1.793e-009 -8.716 -8.746 -0.030

HSO4- 5.578e-012 5.201e-012 -11.254 -11.284 -0.030

CaHSO4+ 4.165e-014 3.883e-014 -13.380 -13.411 -0.030

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.94 -7.33 -4.39 CaSO4

Aragonite 1.33 -7.04 -8.37 CaCO3

Calcite 1.47 -7.04 -8.51 CaCO3

CO2(g) -4.10 -5.63 -1.53 CO2

Dolomite 2.87 -14.35 -17.22 CaMg(CO3)2

Gypsum -2.75 -7.33 -4.58 CaSO4:2H2O

H2(g) -26.40 -29.57 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.30 1.59 NaCl

O2(g) -0.37 -3.30 -2.93 O2

Initial solution 22. 29/8/2012 17:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.773e-003 2.773e-003

Ca 1.014e-003 1.014e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.005e-003 1.005e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.210

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 290

Density (g/cm3) = 0.99573

Activity of water = 1.000

Ionic strength = 4.113e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.326e-003

Total CO2 (mol/kg) = 2.326e-003

Temperature (deg C) = 30.390

Electrical balance (eq) = 1.646e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.32

Iterations = 6

Total H = 1.110144e+002

Total O = 5.551469e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.0468 0.6653

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.590e-005 2.413e-005 -4.587 -4.617 -0.031

H+ 6.572e-010 6.166e-010 -9.182 -9.210 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.326e-003

HCO3- 1.881e-003 1.757e-003 -2.726 -2.755 -0.030

CO3-2 1.942e-004 1.478e-004 -3.712 -3.830 -0.118

CaCO3 1.731e-004 1.732e-004 -3.762 -3.761 0.000

MgCO3 5.234e-005 5.239e-005 -4.281 -4.281 0.000

CaHCO3+ 1.601e-005 1.495e-005 -4.796 -4.825 -0.030

MgHCO3+ 7.741e-006 7.219e-006 -5.111 -5.142 -0.030

CO2 2.295e-006 2.298e-006 -5.639 -5.639 0.000

NaCO3- 3.582e-008 3.341e-008 -7.446 -7.476 -0.030

NaHCO3 9.170e-009 9.178e-009 -8.038 -8.037 0.000

Ca 1.014e-003

Ca+2 8.147e-004 6.200e-004 -3.089 -3.208 -0.119

CaCO3 1.731e-004 1.732e-004 -3.762 -3.761 0.000

CaHCO3+ 1.601e-005 1.495e-005 -4.796 -4.825 -0.030

CaSO4 9.739e-006 9.748e-006 -5.012 -5.011 0.000

CaOH+ 1.789e-007 1.669e-007 -6.747 -6.778 -0.030

CaHSO4+ 4.053e-014 3.779e-014 -13.392 -13.423 -0.030

Cl 5.727e-005

Cl- 5.727e-005 5.337e-005 -4.242 -4.273 -0.031

H(0) 5.102e-030

H2 2.551e-030 2.553e-030 -29.593 -29.593 0.000

K 3.325e-006

K+ 3.324e-006 3.097e-006 -5.478 -5.509 -0.031

KSO4- 1.920e-009 1.790e-009 -8.717 -8.747 -0.030

KOH 1.740e-011 1.742e-011 -10.759 -10.759 0.000

Mg 5.184e-004

Mg+2 4.479e-004 3.419e-004 -3.349 -3.466 -0.117

MgCO3 5.234e-005 5.239e-005 -4.281 -4.281 0.000

MgHCO3+ 7.741e-006 7.219e-006 -5.111 -5.142 -0.030

MgSO4 6.882e-006 6.889e-006 -5.162 -5.162 0.000

MgOH+ 3.482e-006 3.247e-006 -5.458 -5.489 -0.030

Na 1.001e-005

Na+ 9.958e-006 9.291e-006 -5.002 -5.032 -0.030

NaCO3- 3.582e-008 3.341e-008 -7.446 -7.476 -0.030

NaHCO3 9.170e-009 9.178e-009 -8.038 -8.037 0.000

NaSO4- 3.873e-009 3.611e-009 -8.412 -8.442 -0.030

NaOH 9.946e-011 9.955e-011 -10.002 -10.002 0.000

O(0) 1.005e-003

O2 5.026e-004 5.031e-004 -3.299 -3.298 0.000

S(6) 1.154e-004

SO4-2 9.874e-005 7.500e-005 -4.005 -4.125 -0.119

CaSO4 9.739e-006 9.748e-006 -5.012 -5.011 0.000

MgSO4 6.882e-006 6.889e-006 -5.162 -5.162 0.000

NaSO4- 3.873e-009 3.611e-009 -8.412 -8.442 -0.030

KSO4- 1.920e-009 1.790e-009 -8.717 -8.747 -0.030

HSO4- 5.437e-012 5.070e-012 -11.265 -11.295 -0.030

CaHSO4+ 4.053e-014 3.779e-014 -13.392 -13.423 -0.030

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.94 -7.33 -4.39 CaSO4

Aragonite 1.33 -7.04 -8.37 CaCO3

Calcite 1.47 -7.04 -8.51 CaCO3

CO2(g) -4.11 -5.64 -1.53 CO2

Dolomite 2.88 -14.33 -17.21 CaMg(CO3)2

Gypsum -2.75 -7.33 -4.58 CaSO4:2H2O

H2(g) -26.42 -29.59 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.30 1.59 NaCl

O2(g) -0.37 -3.30 -2.93 O2

Initial solution 23. 29/8/2012 17:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.783e-003 2.783e-003

Ca 1.017e-003 1.017e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.009e-003 1.009e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.240

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 289

Density (g/cm3) = 0.99579

Activity of water = 1.000

Ionic strength = 4.108e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.315e-003

Total CO2 (mol/kg) = 2.315e-003

Temperature (deg C) = 30.200

Electrical balance (eq) = 1.362e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.27

Iterations = 6

Total H = 1.110143e+002

Total O = 5.551466e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.0324 0.6640

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.738e-005 2.551e-005 -4.563 -4.593 -0.031

H+ 6.133e-010 5.754e-010 -9.212 -9.240 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.315e-003

HCO3- 1.851e-003 1.729e-003 -2.733 -2.762 -0.030

CO3-2 2.040e-004 1.554e-004 -3.690 -3.809 -0.118

CaCO3 1.804e-004 1.806e-004 -3.744 -3.743 0.000

MgCO3 5.460e-005 5.465e-005 -4.263 -4.262 0.000

CaHCO3+ 1.566e-005 1.463e-005 -4.805 -4.835 -0.030

MgHCO3+ 7.575e-006 7.064e-006 -5.121 -5.151 -0.030

CO2 2.112e-006 2.114e-006 -5.675 -5.675 0.000

NaCO3- 3.730e-008 3.479e-008 -7.428 -7.459 -0.030

NaHCO3 9.024e-009 9.033e-009 -8.045 -8.044 0.000

Ca 1.017e-003

Ca+2 8.115e-004 6.177e-004 -3.091 -3.209 -0.119

CaCO3 1.804e-004 1.806e-004 -3.744 -3.743 0.000

CaHCO3+ 1.566e-005 1.463e-005 -4.805 -4.835 -0.030

CaSO4 9.698e-006 9.707e-006 -5.013 -5.013 0.000

CaOH+ 1.910e-007 1.781e-007 -6.719 -6.749 -0.030

CaHSO4+ 3.756e-014 3.503e-014 -13.425 -13.456 -0.030

Cl 5.727e-005

Cl- 5.727e-005 5.337e-005 -4.242 -4.273 -0.031

H(0) 4.452e-030

H2 2.226e-030 2.228e-030 -29.653 -29.652 0.000

K 3.325e-006

K+ 3.324e-006 3.097e-006 -5.478 -5.509 -0.031

KSO4- 1.916e-009 1.787e-009 -8.718 -8.748 -0.030

KOH 1.864e-011 1.866e-011 -10.729 -10.729 0.000

Mg 5.184e-004

Mg+2 4.457e-004 3.403e-004 -3.351 -3.468 -0.117

MgCO3 5.460e-005 5.465e-005 -4.263 -4.262 0.000

MgHCO3+ 7.575e-006 7.064e-006 -5.121 -5.151 -0.030

MgSO4 6.826e-006 6.832e-006 -5.166 -5.165 0.000

MgOH+ 3.652e-006 3.406e-006 -5.437 -5.468 -0.030

Na 1.001e-005

Na+ 9.957e-006 9.291e-006 -5.002 -5.032 -0.030

NaCO3- 3.730e-008 3.479e-008 -7.428 -7.459 -0.030

NaHCO3 9.024e-009 9.033e-009 -8.045 -8.044 0.000

NaSO4- 3.873e-009 3.612e-009 -8.412 -8.442 -0.030

NaOH 1.066e-010 1.067e-010 -9.972 -9.972 0.000

O(0) 1.009e-003

O2 5.045e-004 5.050e-004 -3.297 -3.297 0.000

S(6) 1.154e-004

SO4-2 9.884e-005 7.509e-005 -4.005 -4.124 -0.119

CaSO4 9.698e-006 9.707e-006 -5.013 -5.013 0.000

MgSO4 6.826e-006 6.832e-006 -5.166 -5.165 0.000

NaSO4- 3.873e-009 3.612e-009 -8.412 -8.442 -0.030

KSO4- 1.916e-009 1.787e-009 -8.718 -8.748 -0.030

HSO4- 5.058e-012 4.717e-012 -11.296 -11.326 -0.030

CaHSO4+ 3.756e-014 3.503e-014 -13.425 -13.456 -0.030

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.95 -7.33 -4.39 CaSO4

Aragonite 1.35 -7.02 -8.37 CaCO3

Calcite 1.49 -7.02 -8.51 CaCO3

CO2(g) -4.15 -5.67 -1.53 CO2

Dolomite 2.91 -14.29 -17.21 CaMg(CO3)2

Gypsum -2.75 -7.33 -4.58 CaSO4:2H2O

H2(g) -26.48 -29.65 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.30 1.59 NaCl

O2(g) -0.37 -3.30 -2.93 O2

Initial solution 24. 29/8/2012 17:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.783e-003 2.783e-003

Ca 1.017e-003 1.017e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.027e-003 1.027e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.250

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 288

Density (g/cm3) = 0.99584

Activity of water = 1.000

Ionic strength = 4.105e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.310e-003

Total CO2 (mol/kg) = 2.310e-003

Temperature (deg C) = 30.030

Electrical balance (eq) = 1.362e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.27

Iterations = 6

Total H = 1.110143e+002

Total O = 5.551466e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.0380 0.6640

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.767e-005 2.579e-005 -4.558 -4.589 -0.031

H+ 5.993e-010 5.623e-010 -9.222 -9.250 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.310e-003

HCO3- 1.840e-003 1.719e-003 -2.735 -2.765 -0.030

CO3-2 2.070e-004 1.577e-004 -3.684 -3.802 -0.118

CaCO3 1.820e-004 1.822e-004 -3.740 -3.739 0.000

MgCO3 5.519e-005 5.525e-005 -4.258 -4.258 0.000

CaHCO3+ 1.551e-005 1.449e-005 -4.809 -4.839 -0.030

MgHCO3+ 7.518e-006 7.011e-006 -5.124 -5.154 -0.030

CO2 2.056e-006 2.058e-006 -5.687 -5.687 0.000

NaCO3- 3.753e-008 3.500e-008 -7.426 -7.456 -0.030

NaHCO3 8.974e-009 8.983e-009 -8.047 -8.047 0.000

Ca 1.017e-003

Ca+2 8.101e-004 6.167e-004 -3.091 -3.210 -0.118

CaCO3 1.820e-004 1.822e-004 -3.740 -3.739 0.000

CaHCO3+ 1.551e-005 1.449e-005 -4.809 -4.839 -0.030

CaSO4 9.674e-006 9.683e-006 -5.014 -5.014 0.000

CaOH+ 1.951e-007 1.820e-007 -6.710 -6.740 -0.030

CaHSO4+ 3.653e-014 3.407e-014 -13.437 -13.468 -0.030

Cl 5.727e-005

Cl- 5.727e-005 5.338e-005 -4.242 -4.273 -0.031

H(0) 4.258e-030

H2 2.129e-030 2.131e-030 -29.672 -29.671 0.000

K 3.325e-006

K+ 3.324e-006 3.097e-006 -5.478 -5.509 -0.031

KSO4- 1.912e-009 1.783e-009 -8.719 -8.749 -0.030

KOH 1.908e-011 1.910e-011 -10.719 -10.719 0.000

Mg 5.184e-004

Mg+2 4.452e-004 3.399e-004 -3.351 -3.469 -0.117

MgCO3 5.519e-005 5.525e-005 -4.258 -4.258 0.000

MgHCO3+ 7.518e-006 7.011e-006 -5.124 -5.154 -0.030

MgSO4 6.795e-006 6.802e-006 -5.168 -5.167 0.000

MgOH+ 3.678e-006 3.430e-006 -5.434 -5.465 -0.030

Na 1.001e-005

Na+ 9.956e-006 9.291e-006 -5.002 -5.032 -0.030

NaCO3- 3.753e-008 3.500e-008 -7.426 -7.456 -0.030

NaHCO3 8.974e-009 8.983e-009 -8.047 -8.047 0.000

NaSO4- 3.871e-009 3.610e-009 -8.412 -8.442 -0.030

NaOH 1.090e-010 1.091e-010 -9.962 -9.962 0.000

O(0) 1.027e-003

O2 5.136e-004 5.141e-004 -3.289 -3.289 0.000

S(6) 1.154e-004

SO4-2 9.889e-005 7.514e-005 -4.005 -4.124 -0.119

CaSO4 9.674e-006 9.683e-006 -5.014 -5.014 0.000

MgSO4 6.795e-006 6.802e-006 -5.168 -5.167 0.000

NaSO4- 3.871e-009 3.610e-009 -8.412 -8.442 -0.030

KSO4- 1.912e-009 1.783e-009 -8.719 -8.749 -0.030

HSO4- 4.927e-012 4.595e-012 -11.307 -11.338 -0.030

CaHSO4+ 3.653e-014 3.407e-014 -13.437 -13.468 -0.030

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.95 -7.33 -4.39 CaSO4

Aragonite 1.36 -7.01 -8.37 CaCO3

Calcite 1.50 -7.01 -8.51 CaCO3

CO2(g) -4.16 -5.69 -1.52 CO2

Dolomite 2.92 -14.28 -17.20 CaMg(CO3)2

Gypsum -2.75 -7.33 -4.58 CaSO4:2H2O

H2(g) -26.50 -29.67 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.30 1.59 NaCl

O2(g) -0.36 -3.29 -2.93 O2

Initial solution 25. 29/8/2012 17:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.773e-003 2.773e-003

Ca 1.014e-003 1.014e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.001e-003 1.001e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.280

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 285

Density (g/cm3) = 0.99590

Activity of water = 1.000

Ionic strength = 4.082e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.282e-003

Total CO2 (mol/kg) = 2.282e-003

Temperature (deg C) = 29.810

Electrical balance (eq) = 1.646e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.33

Iterations = 6

Total H = 1.110143e+002

Total O = 5.551456e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.0228 0.6626

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.918e-005 2.720e-005 -4.535 -4.565 -0.031

H+ 5.592e-010 5.248e-010 -9.252 -9.280 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.282e-003

HCO3- 1.798e-003 1.680e-003 -2.745 -2.775 -0.029

CO3-2 2.157e-004 1.644e-004 -3.666 -3.784 -0.118

CaCO3 1.871e-004 1.873e-004 -3.728 -3.728 0.000

MgCO3 5.716e-005 5.722e-005 -4.243 -4.242 0.000

CaHCO3+ 1.497e-005 1.399e-005 -4.825 -4.854 -0.029

MgHCO3+ 7.309e-006 6.818e-006 -5.136 -5.166 -0.030

CO2 1.878e-006 1.880e-006 -5.726 -5.726 0.000

NaCO3- 3.872e-008 3.612e-008 -7.412 -7.442 -0.030

NaHCO3 8.769e-009 8.777e-009 -8.057 -8.057 0.000

Ca 1.014e-003

Ca+2 8.019e-004 6.110e-004 -3.096 -3.214 -0.118

CaCO3 1.871e-004 1.873e-004 -3.728 -3.728 0.000

CaHCO3+ 1.497e-005 1.399e-005 -4.825 -4.854 -0.029

CaSO4 9.586e-006 9.595e-006 -5.018 -5.018 0.000

CaOH+ 2.071e-007 1.932e-007 -6.684 -6.714 -0.030

CaHSO4+ 3.367e-014 3.141e-014 -13.473 -13.503 -0.030

Cl 5.727e-005

Cl- 5.727e-005 5.339e-005 -4.242 -4.273 -0.031

H(0) 3.717e-030

H2 1.858e-030 1.860e-030 -29.731 -29.730 0.000

K 3.325e-006

K+ 3.324e-006 3.098e-006 -5.478 -5.509 -0.031

KSO4- 1.909e-009 1.780e-009 -8.719 -8.749 -0.030

KOH 2.045e-011 2.047e-011 -10.689 -10.689 0.000

Mg 5.184e-004

Mg+2 4.433e-004 3.388e-004 -3.353 -3.470 -0.117

MgCO3 5.716e-005 5.722e-005 -4.243 -4.242 0.000

MgHCO3+ 7.309e-006 6.818e-006 -5.136 -5.166 -0.030

MgSO4 6.749e-006 6.756e-006 -5.171 -5.170 0.000

MgOH+ 3.852e-006 3.593e-006 -5.414 -5.445 -0.030

Na 1.001e-005

Na+ 9.955e-006 9.292e-006 -5.002 -5.032 -0.030

NaCO3- 3.872e-008 3.612e-008 -7.412 -7.442 -0.030

NaHCO3 8.769e-009 8.777e-009 -8.057 -8.057 0.000

NaSO4- 3.874e-009 3.614e-009 -8.412 -8.442 -0.030

NaOH 1.169e-010 1.170e-010 -9.932 -9.932 0.000

O(0) 1.001e-003

O2 5.004e-004 5.009e-004 -3.301 -3.300 0.000

S(6) 1.154e-004

SO4-2 9.903e-005 7.531e-005 -4.004 -4.123 -0.119

CaSO4 9.586e-006 9.595e-006 -5.018 -5.018 0.000

MgSO4 6.749e-006 6.756e-006 -5.171 -5.170 0.000

NaSO4- 3.874e-009 3.614e-009 -8.412 -8.442 -0.030

KSO4- 1.909e-009 1.780e-009 -8.719 -8.749 -0.030

HSO4- 4.584e-012 4.276e-012 -11.339 -11.369 -0.030

CaHSO4+ 3.367e-014 3.141e-014 -13.473 -13.503 -0.030

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.95 -7.34 -4.38 CaSO4

Aragonite 1.37 -7.00 -8.37 CaCO3

Calcite 1.51 -7.00 -8.51 CaCO3

CO2(g) -4.20 -5.73 -1.52 CO2

Dolomite 2.95 -14.25 -17.20 CaMg(CO3)2

Gypsum -2.75 -7.34 -4.58 CaSO4:2H2O

H2(g) -26.56 -29.73 -3.17 H2

H2O(g) -1.39 -0.00 1.39 H2O

Halite -10.90 -9.30 1.59 NaCl

O2(g) -0.37 -3.30 -2.93 O2

Initial solution 26. 29/8/2012 18:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.732e-003 2.732e-003

Ca 9.988e-004 9.988e-004

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.946e-004 9.946e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.310

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 280

Density (g/cm3) = 0.99595

Activity of water = 1.000

Ionic strength = 4.030e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.229e-003

Total CO2 (mol/kg) = 2.229e-003

Temperature (deg C) = 29.630

Electrical balance (eq) = 2.765e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.56

Iterations = 6

Total H = 1.110142e+002

Total O = 5.551439e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.0066 0.6612

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.085e-005 2.877e-005 -4.511 -4.541 -0.030

H+ 5.217e-010 4.898e-010 -9.283 -9.310 -0.027

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.229e-003

HCO3- 1.736e-003 1.623e-003 -2.760 -2.790 -0.029

CO3-2 2.222e-004 1.697e-004 -3.653 -3.770 -0.117

CaCO3 1.888e-004 1.890e-004 -3.724 -3.724 0.000

MgCO3 5.873e-005 5.878e-005 -4.231 -4.231 0.000

CaHCO3+ 1.417e-005 1.324e-005 -4.849 -4.878 -0.029

MgHCO3+ 7.039e-006 6.569e-006 -5.152 -5.182 -0.030

CO2 1.697e-006 1.698e-006 -5.770 -5.770 0.000

NaCO3- 3.960e-008 3.696e-008 -7.402 -7.432 -0.030

NaHCO3 8.475e-009 8.483e-009 -8.072 -8.071 0.000

Ca 9.988e-004

Ca+2 7.861e-004 5.999e-004 -3.105 -3.222 -0.117

CaCO3 1.888e-004 1.890e-004 -3.724 -3.724 0.000

CaHCO3+ 1.417e-005 1.324e-005 -4.849 -4.878 -0.029

CaSO4 9.430e-006 9.439e-006 -5.025 -5.025 0.000

CaOH+ 2.178e-007 2.033e-007 -6.662 -6.692 -0.030

CaHSO4+ 3.083e-014 2.877e-014 -13.511 -13.541 -0.030

Cl 5.727e-005

Cl- 5.727e-005 5.341e-005 -4.242 -4.272 -0.030

H(0) 3.243e-030

H2 1.621e-030 1.623e-030 -29.790 -29.790 0.000

K 3.325e-006

K+ 3.324e-006 3.099e-006 -5.478 -5.509 -0.030

KSO4- 1.909e-009 1.782e-009 -8.719 -8.749 -0.030

KOH 2.192e-011 2.194e-011 -10.659 -10.659 0.000

Mg 5.184e-004

Mg+2 4.418e-004 3.382e-004 -3.355 -3.471 -0.116

MgCO3 5.873e-005 5.878e-005 -4.231 -4.231 0.000

MgHCO3+ 7.039e-006 6.569e-006 -5.152 -5.182 -0.030

MgSO4 6.730e-006 6.737e-006 -5.172 -5.172 0.000

MgOH+ 4.054e-006 3.784e-006 -5.392 -5.422 -0.030

Na 1.001e-005

Na+ 9.955e-006 9.295e-006 -5.002 -5.032 -0.030

NaCO3- 3.960e-008 3.696e-008 -7.402 -7.432 -0.030

NaHCO3 8.475e-009 8.483e-009 -8.072 -8.071 0.000

NaSO4- 3.883e-009 3.623e-009 -8.411 -8.441 -0.030

NaOH 1.253e-010 1.254e-010 -9.902 -9.902 0.000

O(0) 9.946e-004

O2 4.973e-004 4.978e-004 -3.303 -3.303 0.000

S(6) 1.154e-004

SO4-2 9.920e-005 7.556e-005 -4.003 -4.122 -0.118

CaSO4 9.430e-006 9.439e-006 -5.025 -5.025 0.000

MgSO4 6.730e-006 6.737e-006 -5.172 -5.172 0.000

NaSO4- 3.883e-009 3.623e-009 -8.411 -8.441 -0.030

KSO4- 1.909e-009 1.782e-009 -8.719 -8.749 -0.030

HSO4- 4.274e-012 3.988e-012 -11.369 -11.399 -0.030

CaHSO4+ 3.083e-014 2.877e-014 -13.511 -13.541 -0.030

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.96 -7.34 -4.38 CaSO4

Aragonite 1.37 -6.99 -8.37 CaCO3

Calcite 1.52 -6.99 -8.51 CaCO3

CO2(g) -4.25 -5.77 -1.52 CO2

Dolomite 2.96 -14.23 -17.20 CaMg(CO3)2

Gypsum -2.76 -7.34 -4.58 CaSO4:2H2O

H2(g) -26.62 -29.79 -3.17 H2

H2O(g) -1.39 -0.00 1.39 H2O

Halite -10.90 -9.30 1.59 NaCl

O2(g) -0.38 -3.30 -2.92 O2

Initial solution 27. 29/8/2012 18:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.732e-003 2.732e-003

Ca 9.988e-004 9.988e-004

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.896e-004 9.896e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.280

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 280

Density (g/cm3) = 0.99602

Activity of water = 1.000

Ionic strength = 4.051e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.253e-003

Total CO2 (mol/kg) = 2.253e-003

Temperature (deg C) = 29.420

Electrical balance (eq) = 2.765e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.55

Iterations = 6

Total H = 1.110143e+002

Total O = 5.551446e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.0529 0.6635

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.836e-005 2.644e-005 -4.547 -4.578 -0.030

H+ 5.591e-010 5.248e-010 -9.253 -9.280 -0.027

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.253e-003

HCO3- 1.780e-003 1.664e-003 -2.750 -2.779 -0.029

CO3-2 2.119e-004 1.617e-004 -3.674 -3.791 -0.117

CaCO3 1.807e-004 1.809e-004 -3.743 -3.743 0.000

MgCO3 5.611e-005 5.617e-005 -4.251 -4.251 0.000

CaHCO3+ 1.462e-005 1.366e-005 -4.835 -4.864 -0.029

MgHCO3+ 7.251e-006 6.765e-006 -5.140 -5.170 -0.030

CO2 1.868e-006 1.870e-006 -5.729 -5.728 0.000

NaCO3- 3.737e-008 3.487e-008 -7.427 -7.458 -0.030

NaHCO3 8.689e-009 8.698e-009 -8.061 -8.061 0.000

Ca 9.988e-004

Ca+2 7.937e-004 6.054e-004 -3.100 -3.218 -0.118

CaCO3 1.807e-004 1.809e-004 -3.743 -3.743 0.000

CaHCO3+ 1.462e-005 1.366e-005 -4.835 -4.864 -0.029

CaSO4 9.487e-006 9.496e-006 -5.023 -5.022 0.000

CaOH+ 2.052e-007 1.914e-007 -6.688 -6.718 -0.030

CaHSO4+ 3.314e-014 3.092e-014 -13.480 -13.510 -0.030

Cl 5.727e-005

Cl- 5.727e-005 5.340e-005 -4.242 -4.272 -0.030

H(0) 3.731e-030

H2 1.865e-030 1.867e-030 -29.729 -29.729 0.000

K 3.325e-006

K+ 3.324e-006 3.099e-006 -5.478 -5.509 -0.030

KSO4- 1.901e-009 1.773e-009 -8.721 -8.751 -0.030

KOH 2.045e-011 2.047e-011 -10.689 -10.689 0.000

Mg 5.184e-004

Mg+2 4.446e-004 3.401e-004 -3.352 -3.468 -0.116

MgCO3 5.611e-005 5.617e-005 -4.251 -4.251 0.000

MgHCO3+ 7.251e-006 6.765e-006 -5.140 -5.170 -0.030

MgSO4 6.726e-006 6.732e-006 -5.172 -5.172 0.000

MgOH+ 3.736e-006 3.486e-006 -5.428 -5.458 -0.030

Na 1.001e-005

Na+ 9.957e-006 9.296e-006 -5.002 -5.032 -0.030

NaCO3- 3.737e-008 3.487e-008 -7.427 -7.458 -0.030

NaHCO3 8.689e-009 8.698e-009 -8.061 -8.061 0.000

NaSO4- 3.874e-009 3.615e-009 -8.412 -8.442 -0.030

NaOH 1.169e-010 1.170e-010 -9.932 -9.932 0.000

O(0) 9.896e-004

O2 4.948e-004 4.953e-004 -3.306 -3.305 0.000

S(6) 1.154e-004

SO4-2 9.915e-005 7.548e-005 -4.004 -4.122 -0.118

CaSO4 9.487e-006 9.496e-006 -5.023 -5.022 0.000

MgSO4 6.726e-006 6.732e-006 -5.172 -5.172 0.000

NaSO4- 3.874e-009 3.615e-009 -8.412 -8.442 -0.030

KSO4- 1.901e-009 1.773e-009 -8.721 -8.751 -0.030

HSO4- 4.553e-012 4.249e-012 -11.342 -11.372 -0.030

CaHSO4+ 3.314e-014 3.092e-014 -13.480 -13.510 -0.030

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.96 -7.34 -4.38 CaSO4

Aragonite 1.36 -7.01 -8.37 CaCO3

Calcite 1.50 -7.01 -8.51 CaCO3

CO2(g) -4.21 -5.73 -1.52 CO2

Dolomite 2.92 -14.27 -17.19 CaMg(CO3)2

Gypsum -2.76 -7.34 -4.58 CaSO4:2H2O

H2(g) -26.56 -29.73 -3.17 H2

H2O(g) -1.40 -0.00 1.40 H2O

Halite -10.90 -9.30 1.59 NaCl

O2(g) -0.38 -3.31 -2.92 O2

Initial solution 28. 29/8/2012 18:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.752e-003 2.752e-003

Ca 1.006e-003 1.006e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.865e-004 9.865e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.250

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 281

Density (g/cm3) = 0.99608

Activity of water = 1.000

Ionic strength = 4.091e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.293e-003

Total CO2 (mol/kg) = 2.293e-003

Temperature (deg C) = 29.200

Electrical balance (eq) = 2.214e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.44

Iterations = 6

Total H = 1.110143e+002

Total O = 5.551457e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.1003 0.6659

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.606e-005 2.429e-005 -4.584 -4.615 -0.031

H+ 5.992e-010 5.623e-010 -9.222 -9.250 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.293e-003

HCO3- 1.836e-003 1.715e-003 -2.736 -2.766 -0.029

CO3-2 2.033e-004 1.550e-004 -3.692 -3.810 -0.118

CaCO3 1.749e-004 1.751e-004 -3.757 -3.757 0.000

MgCO3 5.383e-005 5.388e-005 -4.269 -4.269 0.000

CaHCO3+ 1.526e-005 1.426e-005 -4.817 -4.846 -0.029

MgHCO3+ 7.501e-006 6.997e-006 -5.125 -5.155 -0.030

CO2 2.068e-006 2.070e-006 -5.684 -5.684 0.000

NaCO3- 3.544e-008 3.306e-008 -7.451 -7.481 -0.030

NaHCO3 8.958e-009 8.966e-009 -8.048 -8.047 0.000

Ca 1.006e-003

Ca+2 8.063e-004 6.143e-004 -3.094 -3.212 -0.118

CaCO3 1.749e-004 1.751e-004 -3.757 -3.757 0.000

CaHCO3+ 1.526e-005 1.426e-005 -4.817 -4.846 -0.029

CaSO4 9.590e-006 9.599e-006 -5.018 -5.018 0.000

CaOH+ 1.944e-007 1.813e-007 -6.711 -6.742 -0.030

CaHSO4+ 3.580e-014 3.339e-014 -13.446 -13.476 -0.030

Cl 5.727e-005

Cl- 5.727e-005 5.339e-005 -4.242 -4.273 -0.031

H(0) 4.293e-030

H2 2.146e-030 2.148e-030 -29.668 -29.668 0.000

K 3.325e-006

K+ 3.324e-006 3.098e-006 -5.478 -5.509 -0.031

KSO4- 1.890e-009 1.763e-009 -8.724 -8.754 -0.030

KOH 1.908e-011 1.910e-011 -10.719 -10.719 0.000

Mg 5.184e-004

Mg+2 4.469e-004 3.415e-004 -3.350 -3.467 -0.117

MgCO3 5.383e-005 5.388e-005 -4.269 -4.269 0.000

MgHCO3+ 7.501e-006 6.997e-006 -5.125 -5.155 -0.030

MgSO4 6.704e-006 6.711e-006 -5.174 -5.173 0.000

MgOH+ 3.436e-006 3.205e-006 -5.464 -5.494 -0.030

Na 1.001e-005

Na+ 9.959e-006 9.295e-006 -5.002 -5.032 -0.030

NaCO3- 3.544e-008 3.306e-008 -7.451 -7.481 -0.030

NaHCO3 8.958e-009 8.966e-009 -8.048 -8.047 0.000

NaSO4- 3.862e-009 3.603e-009 -8.413 -8.443 -0.030

NaOH 1.091e-010 1.092e-010 -9.962 -9.962 0.000

O(0) 9.865e-004

O2 4.932e-004 4.937e-004 -3.307 -3.307 0.000

S(6) 1.154e-004

SO4-2 9.907e-005 7.534e-005 -4.004 -4.123 -0.119

CaSO4 9.590e-006 9.599e-006 -5.018 -5.018 0.000

MgSO4 6.704e-006 6.711e-006 -5.174 -5.173 0.000

NaSO4- 3.862e-009 3.603e-009 -8.413 -8.443 -0.030

KSO4- 1.890e-009 1.763e-009 -8.724 -8.754 -0.030

HSO4- 4.847e-012 4.521e-012 -11.315 -11.345 -0.030

CaHSO4+ 3.580e-014 3.339e-014 -13.446 -13.476 -0.030

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.95 -7.33 -4.38 CaSO4

Aragonite 1.34 -7.02 -8.36 CaCO3

Calcite 1.48 -7.02 -8.50 CaCO3

CO2(g) -4.17 -5.68 -1.52 CO2

Dolomite 2.89 -14.30 -17.19 CaMg(CO3)2

Gypsum -2.75 -7.33 -4.58 CaSO4:2H2O

H2(g) -26.50 -29.67 -3.17 H2

H2O(g) -1.40 -0.00 1.40 H2O

Halite -10.90 -9.30 1.59 NaCl

O2(g) -0.39 -3.31 -2.92 O2

Initial solution 29. 29/8/2012 18:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.752e-003 2.752e-003

Ca 1.006e-003 1.006e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.815e-004 9.815e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.210

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 282

Density (g/cm3) = 0.99614

Activity of water = 1.000

Ionic strength = 4.116e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.322e-003

Total CO2 (mol/kg) = 2.322e-003

Temperature (deg C) = 29.020

Electrical balance (eq) = 2.214e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.43

Iterations = 6

Total H = 1.110144e+002

Total O = 5.551465e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.1542 0.6687

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.346e-005 2.187e-005 -4.630 -4.660 -0.031

H+ 6.571e-010 6.166e-010 -9.182 -9.210 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.322e-003

HCO3- 1.890e-003 1.766e-003 -2.723 -2.753 -0.030

CO3-2 1.904e-004 1.451e-004 -3.720 -3.838 -0.118

CaCO3 1.648e-004 1.650e-004 -3.783 -3.783 0.000

MgCO3 5.057e-005 5.062e-005 -4.296 -4.296 0.000

CaHCO3+ 1.585e-005 1.480e-005 -4.800 -4.830 -0.030

MgHCO3+ 7.768e-006 7.245e-006 -5.110 -5.140 -0.030

CO2 2.339e-006 2.341e-006 -5.631 -5.631 0.000

NaCO3- 3.288e-008 3.067e-008 -7.483 -7.513 -0.030

NaHCO3 9.223e-009 9.232e-009 -8.035 -8.035 0.000

Ca 1.006e-003

Ca+2 8.157e-004 6.211e-004 -3.088 -3.207 -0.118

CaCO3 1.648e-004 1.650e-004 -3.783 -3.783 0.000

CaHCO3+ 1.585e-005 1.480e-005 -4.800 -4.830 -0.030

CaSO4 9.665e-006 9.674e-006 -5.015 -5.014 0.000

CaOH+ 1.792e-007 1.672e-007 -6.747 -6.777 -0.030

CaHSO4+ 3.947e-014 3.681e-014 -13.404 -13.434 -0.030

Cl 5.727e-005

Cl- 5.727e-005 5.338e-005 -4.242 -4.273 -0.031

H(0) 5.170e-030

H2 2.585e-030 2.587e-030 -29.588 -29.587 0.000

K 3.325e-006

K+ 3.324e-006 3.098e-006 -5.478 -5.509 -0.031

KSO4- 1.881e-009 1.755e-009 -8.726 -8.756 -0.030

KOH 1.740e-011 1.742e-011 -10.759 -10.759 0.000

Mg 5.184e-004

Mg+2 4.502e-004 3.438e-004 -3.347 -3.464 -0.117

MgCO3 5.057e-005 5.062e-005 -4.296 -4.296 0.000

MgHCO3+ 7.768e-006 7.245e-006 -5.110 -5.140 -0.030

MgSO4 6.709e-006 6.715e-006 -5.173 -5.173 0.000

MgOH+ 3.106e-006 2.896e-006 -5.508 -5.538 -0.030

Na 1.001e-005

Na+ 9.961e-006 9.295e-006 -5.002 -5.032 -0.030

NaCO3- 3.288e-008 3.067e-008 -7.483 -7.513 -0.030

NaHCO3 9.223e-009 9.232e-009 -8.035 -8.035 0.000

NaSO4- 3.853e-009 3.594e-009 -8.414 -8.444 -0.030

NaOH 9.950e-011 9.959e-011 -10.002 -10.002 0.000

O(0) 9.815e-004

O2 4.907e-004 4.912e-004 -3.309 -3.309 0.000

S(6) 1.154e-004

SO4-2 9.899e-005 7.523e-005 -4.004 -4.124 -0.119

CaSO4 9.665e-006 9.674e-006 -5.015 -5.014 0.000

MgSO4 6.709e-006 6.715e-006 -5.173 -5.173 0.000

NaSO4- 3.853e-009 3.594e-009 -8.414 -8.444 -0.030

KSO4- 1.881e-009 1.755e-009 -8.726 -8.756 -0.030

HSO4- 5.286e-012 4.930e-012 -11.277 -11.307 -0.030

CaHSO4+ 3.947e-014 3.681e-014 -13.404 -13.434 -0.030

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.95 -7.33 -4.38 CaSO4

Aragonite 1.32 -7.05 -8.36 CaCO3

Calcite 1.46 -7.05 -8.50 CaCO3

CO2(g) -4.12 -5.63 -1.51 CO2

Dolomite 2.83 -14.35 -17.18 CaMg(CO3)2

Gypsum -2.75 -7.33 -4.58 CaSO4:2H2O

H2(g) -26.42 -29.59 -3.17 H2

H2O(g) -1.41 -0.00 1.41 H2O

Halite -10.90 -9.30 1.59 NaCl

O2(g) -0.39 -3.31 -2.92 O2

Initial solution 30. 29/8/2012 19:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.773e-003 2.773e-003

Ca 1.014e-003 1.014e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.759e-004 9.759e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.130

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 285

Density (g/cm3) = 0.99621

Activity of water = 1.000

Ionic strength = 4.184e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.394e-003

Total CO2 (mol/kg) = 2.394e-003

Temperature (deg C) = 28.760

Electrical balance (eq) = 1.646e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.31

Iterations = 7

Total H = 1.110145e+002

Total O = 5.551486e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.2546 0.6742

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.916e-005 1.785e-005 -4.718 -4.748 -0.031

H+ 7.904e-010 7.413e-010 -9.102 -9.130 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.394e-003

HCO3- 2.006e-003 1.873e-003 -2.698 -2.727 -0.030

CO3-2 1.675e-004 1.274e-004 -3.776 -3.895 -0.119

CaCO3 1.477e-004 1.478e-004 -3.831 -3.830 0.000

MgCO3 4.472e-005 4.476e-005 -4.350 -4.349 0.000

CaHCO3+ 1.720e-005 1.606e-005 -4.764 -4.794 -0.030

MgHCO3+ 8.323e-006 7.759e-006 -5.080 -5.110 -0.031

CO2 2.990e-006 2.993e-006 -5.524 -5.524 0.000

NaCO3- 2.852e-008 2.658e-008 -7.545 -7.575 -0.031

NaHCO3 9.781e-009 9.790e-009 -8.010 -8.009 0.000

Ca 1.014e-003

Ca+2 8.389e-004 6.375e-004 -3.076 -3.196 -0.119

CaCO3 1.477e-004 1.478e-004 -3.831 -3.830 0.000

CaHCO3+ 1.720e-005 1.606e-005 -4.764 -4.794 -0.030

CaSO4 9.858e-006 9.868e-006 -5.006 -5.006 0.000

CaOH+ 1.531e-007 1.427e-007 -6.815 -6.846 -0.031

CaHSO4+ 4.826e-014 4.499e-014 -13.316 -13.347 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.335e-005 -4.242 -4.273 -0.031

H(0) 7.491e-030

H2 3.746e-030 3.749e-030 -29.426 -29.426 0.000

K 3.325e-006

K+ 3.324e-006 3.096e-006 -5.478 -5.509 -0.031

KSO4- 1.866e-009 1.739e-009 -8.729 -8.760 -0.031

KOH 1.447e-011 1.448e-011 -10.840 -10.839 0.000

Mg 5.184e-004

Mg+2 4.561e-004 3.476e-004 -3.341 -3.459 -0.118

MgCO3 4.472e-005 4.476e-005 -4.350 -4.349 0.000

MgHCO3+ 8.323e-006 7.759e-006 -5.080 -5.110 -0.031

MgSO4 6.713e-006 6.719e-006 -5.173 -5.173 0.000

MgOH+ 2.554e-006 2.381e-006 -5.593 -5.623 -0.031

Na 1.001e-005

Na+ 9.965e-006 9.294e-006 -5.002 -5.032 -0.030

NaCO3- 2.852e-008 2.658e-008 -7.545 -7.575 -0.031

NaHCO3 9.781e-009 9.790e-009 -8.010 -8.009 0.000

NaSO4- 3.834e-009 3.574e-009 -8.416 -8.447 -0.031

NaOH 8.275e-011 8.283e-011 -10.082 -10.082 0.000

O(0) 9.759e-004

O2 4.879e-004 4.884e-004 -3.312 -3.311 0.000

S(6) 1.154e-004

SO4-2 9.879e-005 7.493e-005 -4.005 -4.125 -0.120

CaSO4 9.858e-006 9.868e-006 -5.006 -5.006 0.000

MgSO4 6.713e-006 6.719e-006 -5.173 -5.173 0.000

NaSO4- 3.834e-009 3.574e-009 -8.416 -8.447 -0.031

KSO4- 1.866e-009 1.739e-009 -8.729 -8.760 -0.031

HSO4- 6.297e-012 5.870e-012 -11.201 -11.231 -0.031

CaHSO4+ 4.826e-014 4.499e-014 -13.316 -13.347 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.94 -7.32 -4.38 CaSO4

Aragonite 1.27 -7.09 -8.36 CaCO3

Calcite 1.41 -7.09 -8.50 CaCO3

CO2(g) -4.01 -5.52 -1.51 CO2

Dolomite 2.73 -14.44 -17.18 CaMg(CO3)2

Gypsum -2.74 -7.32 -4.58 CaSO4:2H2O

H2(g) -26.26 -29.43 -3.17 H2

H2O(g) -1.41 -0.00 1.41 H2O

Halite -10.90 -9.30 1.59 NaCl

O2(g) -0.39 -3.31 -2.92 O2

Initial solution 31. 29/8/2012 19:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.773e-003 2.773e-003

Ca 1.014e-003 1.014e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.702e-004 9.702e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.110

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 284

Density (g/cm3) = 0.99627

Activity of water = 1.000

Ionic strength = 4.198e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.408e-003

Total CO2 (mol/kg) = 2.408e-003

Temperature (deg C) = 28.570

Electrical balance (eq) = 1.646e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.31

Iterations = 7

Total H = 1.110145e+002

Total O = 5.551489e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.2893 0.6758

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.805e-005 1.681e-005 -4.744 -4.774 -0.031

H+ 8.277e-010 7.762e-010 -9.082 -9.110 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.408e-003

HCO3- 2.032e-003 1.897e-003 -2.692 -2.722 -0.030

CO3-2 1.615e-004 1.228e-004 -3.792 -3.911 -0.119

CaCO3 1.425e-004 1.427e-004 -3.846 -3.846 0.000

MgCO3 4.313e-005 4.317e-005 -4.365 -4.365 0.000

CaHCO3+ 1.748e-005 1.632e-005 -4.757 -4.787 -0.030

MgHCO3+ 8.452e-006 7.878e-006 -5.073 -5.104 -0.031

CO2 3.178e-006 3.181e-006 -5.498 -5.497 0.000

NaCO3- 2.724e-008 2.539e-008 -7.565 -7.595 -0.031

NaHCO3 9.908e-009 9.918e-009 -8.004 -8.004 0.000

Ca 1.014e-003

Ca+2 8.437e-004 6.410e-004 -3.074 -3.193 -0.119

CaCO3 1.425e-004 1.427e-004 -3.846 -3.846 0.000

CaHCO3+ 1.748e-005 1.632e-005 -4.757 -4.787 -0.030

CaSO4 9.890e-006 9.899e-006 -5.005 -5.004 0.000

CaOH+ 1.470e-007 1.370e-007 -6.833 -6.863 -0.031

CaHSO4+ 5.057e-014 4.714e-014 -13.296 -13.327 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.335e-005 -4.242 -4.273 -0.031

H(0) 8.229e-030

H2 4.115e-030 4.119e-030 -29.386 -29.385 0.000

K 3.325e-006

K+ 3.324e-006 3.096e-006 -5.478 -5.509 -0.031

KSO4- 1.859e-009 1.733e-009 -8.731 -8.761 -0.031

KOH 1.381e-011 1.383e-011 -10.860 -10.859 0.000

Mg 5.184e-004

Mg+2 4.577e-004 3.488e-004 -3.339 -3.457 -0.118

MgCO3 4.313e-005 4.317e-005 -4.365 -4.365 0.000

MgHCO3+ 8.452e-006 7.878e-006 -5.073 -5.104 -0.031

MgSO4 6.699e-006 6.706e-006 -5.174 -5.174 0.000

MgOH+ 2.407e-006 2.243e-006 -5.619 -5.649 -0.031

Na 1.001e-005

Na+ 9.966e-006 9.295e-006 -5.001 -5.032 -0.030

NaCO3- 2.724e-008 2.539e-008 -7.565 -7.595 -0.031

NaHCO3 9.908e-009 9.918e-009 -8.004 -8.004 0.000

NaSO4- 3.828e-009 3.568e-009 -8.417 -8.448 -0.031

NaOH 7.903e-011 7.910e-011 -10.102 -10.102 0.000

O(0) 9.702e-004

O2 4.851e-004 4.856e-004 -3.314 -3.314 0.000

S(6) 1.154e-004

SO4-2 9.877e-005 7.489e-005 -4.005 -4.126 -0.120

CaSO4 9.890e-006 9.899e-006 -5.005 -5.004 0.000

MgSO4 6.699e-006 6.706e-006 -5.174 -5.174 0.000

NaSO4- 3.828e-009 3.568e-009 -8.417 -8.448 -0.031

KSO4- 1.859e-009 1.733e-009 -8.731 -8.761 -0.031

HSO4- 6.563e-012 6.117e-012 -11.183 -11.213 -0.031

CaHSO4+ 5.057e-014 4.714e-014 -13.296 -13.327 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.94 -7.32 -4.38 CaSO4

Aragonite 1.26 -7.10 -8.36 CaCO3

Calcite 1.40 -7.10 -8.50 CaCO3

CO2(g) -3.99 -5.50 -1.51 CO2

Dolomite 2.70 -14.47 -17.17 CaMg(CO3)2

Gypsum -2.74 -7.32 -4.58 CaSO4:2H2O

H2(g) -26.22 -29.39 -3.17 H2

H2O(g) -1.42 -0.00 1.42 H2O

Halite -10.89 -9.30 1.59 NaCl

O2(g) -0.40 -3.31 -2.92 O2

Initial solution 32. 29/8/2012 19:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.783e-003 2.783e-003

Ca 1.017e-003 1.017e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.609e-004 9.609e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.030

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 287

Density (g/cm3) = 0.99633

Activity of water = 1.000

Ionic strength = 4.253e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.467e-003

Total CO2 (mol/kg) = 2.467e-003

Temperature (deg C) = 28.360

Electrical balance (eq) = 1.362e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.25

Iterations = 7

Total H = 1.110146e+002

Total O = 5.551505e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.3853 0.6811

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.479e-005 1.377e-005 -4.830 -4.861 -0.031

H+ 9.954e-010 9.333e-010 -9.002 -9.030 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.467e-003

HCO3- 2.131e-003 1.989e-003 -2.671 -2.701 -0.030

CO3-2 1.405e-004 1.066e-004 -3.852 -3.972 -0.120

CaCO3 1.258e-004 1.259e-004 -3.900 -3.900 0.000

MgCO3 3.771e-005 3.775e-005 -4.424 -4.423 0.000

CaHCO3+ 1.866e-005 1.742e-005 -4.729 -4.759 -0.030

MgHCO3+ 8.943e-006 8.332e-006 -5.049 -5.079 -0.031

CO2 4.013e-006 4.017e-006 -5.397 -5.396 0.000

NaCO3- 2.342e-008 2.182e-008 -7.630 -7.661 -0.031

NaHCO3 1.038e-008 1.040e-008 -7.984 -7.983 0.000

Ca 1.017e-003

Ca+2 8.628e-004 6.545e-004 -3.064 -3.184 -0.120

CaCO3 1.258e-004 1.259e-004 -3.900 -3.900 0.000

CaHCO3+ 1.866e-005 1.742e-005 -4.729 -4.759 -0.030

CaSO4 1.005e-005 1.006e-005 -4.998 -4.998 0.000

CaOH+ 1.249e-007 1.164e-007 -6.903 -6.934 -0.031

CaHSO4+ 6.162e-014 5.742e-014 -13.210 -13.241 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.333e-005 -4.242 -4.273 -0.031

H(0) 1.192e-029

H2 5.959e-030 5.965e-030 -29.225 -29.224 0.000

K 3.325e-006

K+ 3.324e-006 3.095e-006 -5.478 -5.509 -0.031

KSO4- 1.846e-009 1.720e-009 -8.734 -8.764 -0.031

KOH 1.149e-011 1.150e-011 -10.940 -10.939 0.000

Mg 5.184e-004

Mg+2 4.630e-004 3.523e-004 -3.334 -3.453 -0.119

MgCO3 3.771e-005 3.775e-005 -4.424 -4.423 0.000

MgHCO3+ 8.943e-006 8.332e-006 -5.049 -5.079 -0.031

MgSO4 6.710e-006 6.717e-006 -5.173 -5.173 0.000

MgOH+ 1.986e-006 1.850e-006 -5.702 -5.733 -0.031

Na 1.001e-005

Na+ 9.969e-006 9.294e-006 -5.001 -5.032 -0.030

NaCO3- 2.342e-008 2.182e-008 -7.630 -7.661 -0.031

NaHCO3 1.038e-008 1.040e-008 -7.984 -7.983 0.000

NaSO4- 3.812e-009 3.551e-009 -8.419 -8.450 -0.031

NaOH 6.573e-011 6.579e-011 -10.182 -10.182 0.000

O(0) 9.609e-004

O2 4.804e-004 4.809e-004 -3.318 -3.318 0.000

S(6) 1.154e-004

SO4-2 9.861e-005 7.465e-005 -4.006 -4.127 -0.121

CaSO4 1.005e-005 1.006e-005 -4.998 -4.998 0.000

MgSO4 6.710e-006 6.717e-006 -5.173 -5.173 0.000

NaSO4- 3.812e-009 3.551e-009 -8.419 -8.450 -0.031

KSO4- 1.846e-009 1.720e-009 -8.734 -8.764 -0.031

HSO4- 7.831e-012 7.296e-012 -11.106 -11.137 -0.031

CaHSO4+ 6.162e-014 5.742e-014 -13.210 -13.241 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.93 -7.31 -4.38 CaSO4

Aragonite 1.20 -7.16 -8.36 CaCO3

Calcite 1.34 -7.16 -8.50 CaCO3

CO2(g) -3.89 -5.40 -1.51 CO2

Dolomite 2.59 -14.58 -17.17 CaMg(CO3)2

Gypsum -2.73 -7.31 -4.58 CaSO4:2H2O

H2(g) -26.06 -29.22 -3.16 H2

H2O(g) -1.42 -0.00 1.42 H2O

Halite -10.89 -9.30 1.59 NaCl

O2(g) -0.40 -3.32 -2.92 O2

Initial solution 33. 29/8/2012 19:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.814e-003 2.814e-003

Ca 1.029e-003 1.029e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.515e-004 9.515e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.950

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 290

Density (g/cm3) = 0.99639

Activity of water = 1.000

Ionic strength = 4.326e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.539e-003

Total CO2 (mol/kg) = 2.539e-003

Temperature (deg C) = 28.160

Electrical balance (eq) = 5.094e-006

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.09

Iterations = 7

Total H = 1.110147e+002

Total O = 5.551525e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.4804 0.6863

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.213e-005 1.129e-005 -4.916 -4.947 -0.031

H+ 1.197e-009 1.122e-009 -8.922 -8.950 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.539e-003

HCO3- 2.237e-003 2.087e-003 -2.650 -2.681 -0.030

CO3-2 1.224e-004 9.272e-005 -3.912 -4.033 -0.121

CaCO3 1.117e-004 1.118e-004 -3.952 -3.952 0.000

MgCO3 3.295e-005 3.298e-005 -4.482 -4.482 0.000

CaHCO3+ 2.004e-005 1.870e-005 -4.698 -4.728 -0.030

MgHCO3+ 9.453e-006 8.803e-006 -5.024 -5.055 -0.031

CO2 5.073e-006 5.078e-006 -5.295 -5.294 0.000

NaCO3- 2.017e-008 1.878e-008 -7.695 -7.726 -0.031

NaHCO3 1.089e-008 1.090e-008 -7.963 -7.962 0.000

Ca 1.029e-003

Ca+2 8.866e-004 6.713e-004 -3.052 -3.173 -0.121

CaCO3 1.117e-004 1.118e-004 -3.952 -3.952 0.000

CaHCO3+ 2.004e-005 1.870e-005 -4.698 -4.728 -0.030

CaSO4 1.024e-005 1.025e-005 -4.990 -4.989 0.000

CaOH+ 1.066e-007 9.928e-008 -6.972 -7.003 -0.031

CaHSO4+ 7.538e-014 7.020e-014 -13.123 -13.154 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.330e-005 -4.242 -4.273 -0.031

H(0) 1.726e-029

H2 8.631e-030 8.639e-030 -29.064 -29.064 0.000

K 3.325e-006

K+ 3.324e-006 3.093e-006 -5.478 -5.510 -0.031

KSO4- 1.833e-009 1.707e-009 -8.737 -8.768 -0.031

KOH 9.548e-012 9.557e-012 -11.020 -11.020 0.000

Mg 5.184e-004

Mg+2 4.677e-004 3.551e-004 -3.330 -3.450 -0.120

MgCO3 3.295e-005 3.298e-005 -4.482 -4.482 0.000

MgHCO3+ 9.453e-006 8.803e-006 -5.024 -5.055 -0.031

MgSO4 6.703e-006 6.709e-006 -5.174 -5.173 0.000

MgOH+ 1.636e-006 1.524e-006 -5.786 -5.817 -0.031

Na 1.001e-005

Na+ 9.972e-006 9.292e-006 -5.001 -5.032 -0.031

NaCO3- 2.017e-008 1.878e-008 -7.695 -7.726 -0.031

NaHCO3 1.089e-008 1.090e-008 -7.963 -7.962 0.000

NaSO4- 3.793e-009 3.532e-009 -8.421 -8.452 -0.031

NaOH 5.466e-011 5.471e-011 -10.262 -10.262 0.000

O(0) 9.515e-004

O2 4.757e-004 4.762e-004 -3.323 -3.322 0.000

S(6) 1.154e-004

SO4-2 9.842e-005 7.436e-005 -4.007 -4.129 -0.122

CaSO4 1.024e-005 1.025e-005 -4.990 -4.989 0.000

MgSO4 6.703e-006 6.709e-006 -5.174 -5.173 0.000

NaSO4- 3.793e-009 3.532e-009 -8.421 -8.452 -0.031

KSO4- 1.833e-009 1.707e-009 -8.737 -8.768 -0.031

HSO4- 9.340e-012 8.698e-012 -11.030 -11.061 -0.031

CaHSO4+ 7.538e-014 7.020e-014 -13.123 -13.154 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.93 -7.30 -4.38 CaSO4

Aragonite 1.15 -7.21 -8.36 CaCO3

Calcite 1.29 -7.21 -8.50 CaCO3

CO2(g) -3.79 -5.29 -1.50 CO2

Dolomite 2.47 -14.69 -17.16 CaMg(CO3)2

Gypsum -2.72 -7.30 -4.58 CaSO4:2H2O

H2(g) -25.90 -29.06 -3.16 H2

H2O(g) -1.43 -0.00 1.43 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.41 -3.32 -2.91 O2

Initial solution 34. 29/8/2012 20:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.814e-003 2.814e-003

Ca 1.029e-003 1.029e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.402e-004 9.402e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.910

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 291

Density (g/cm3) = 0.99644

Activity of water = 1.000

Ionic strength = 4.346e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.560e-003

Total CO2 (mol/kg) = 2.560e-003

Temperature (deg C) = 28.000

Electrical balance (eq) = 5.094e-006

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.09

Iterations = 7

Total H = 1.110148e+002

Total O = 5.551531e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.5321 0.6891

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.094e-005 1.017e-005 -4.961 -4.993 -0.031

H+ 1.313e-009 1.230e-009 -8.882 -8.910 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.560e-003

HCO3- 2.276e-003 2.123e-003 -2.643 -2.673 -0.030

CO3-2 1.133e-004 8.579e-005 -3.946 -4.067 -0.121

CaCO3 1.038e-004 1.039e-004 -3.984 -3.984 0.000

MgCO3 3.055e-005 3.058e-005 -4.515 -4.515 0.000

CaHCO3+ 2.051e-005 1.913e-005 -4.688 -4.718 -0.030

MgHCO3+ 9.656e-006 8.991e-006 -5.015 -5.046 -0.031

CO2 5.670e-006 5.675e-006 -5.246 -5.246 0.000

NaCO3- 1.852e-008 1.724e-008 -7.732 -7.763 -0.031

NaHCO3 1.108e-008 1.110e-008 -7.955 -7.955 0.000

Ca 1.029e-003

Ca+2 8.940e-004 6.765e-004 -3.049 -3.170 -0.121

CaCO3 1.038e-004 1.039e-004 -3.984 -3.984 0.000

CaHCO3+ 2.051e-005 1.913e-005 -4.688 -4.718 -0.030

CaSO4 1.030e-005 1.031e-005 -4.987 -4.987 0.000

CaOH+ 9.800e-008 9.125e-008 -7.009 -7.040 -0.031

CaHSO4+ 8.292e-014 7.721e-014 -13.081 -13.112 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.329e-005 -4.242 -4.273 -0.031

H(0) 2.079e-029

H2 1.039e-029 1.040e-029 -28.983 -28.983 0.000

K 3.325e-006

K+ 3.324e-006 3.092e-006 -5.478 -5.510 -0.031

KSO4- 1.826e-009 1.700e-009 -8.739 -8.770 -0.031

KOH 8.706e-012 8.715e-012 -11.060 -11.060 0.000

Mg 5.184e-004

Mg+2 4.700e-004 3.567e-004 -3.328 -3.448 -0.120

MgCO3 3.055e-005 3.058e-005 -4.515 -4.515 0.000

MgHCO3+ 9.656e-006 8.991e-006 -5.015 -5.046 -0.031

MgSO4 6.699e-006 6.706e-006 -5.174 -5.174 0.000

MgOH+ 1.478e-006 1.377e-006 -5.830 -5.861 -0.031

Na 1.001e-005

Na+ 9.974e-006 9.292e-006 -5.001 -5.032 -0.031

NaCO3- 1.852e-008 1.724e-008 -7.732 -7.763 -0.031

NaHCO3 1.108e-008 1.110e-008 -7.955 -7.955 0.000

NaSO4- 3.786e-009 3.525e-009 -8.422 -8.453 -0.031

NaOH 4.985e-011 4.990e-011 -10.302 -10.302 0.000

O(0) 9.402e-004

O2 4.701e-004 4.706e-004 -3.328 -3.327 0.000

S(6) 1.154e-004

SO4-2 9.837e-005 7.428e-005 -4.007 -4.129 -0.122

CaSO4 1.030e-005 1.031e-005 -4.987 -4.987 0.000

MgSO4 6.699e-006 6.706e-006 -5.174 -5.174 0.000

NaSO4- 3.786e-009 3.525e-009 -8.422 -8.453 -0.031

KSO4- 1.826e-009 1.700e-009 -8.739 -8.770 -0.031

HSO4- 1.020e-011 9.493e-012 -10.992 -11.023 -0.031

CaHSO4+ 8.292e-014 7.721e-014 -13.081 -13.112 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.92 -7.30 -4.37 CaSO4

Aragonite 1.12 -7.24 -8.36 CaCO3

Calcite 1.26 -7.24 -8.50 CaCO3

CO2(g) -3.74 -5.25 -1.50 CO2

Dolomite 2.41 -14.75 -17.16 CaMg(CO3)2

Gypsum -2.72 -7.30 -4.58 CaSO4:2H2O

H2(g) -25.82 -28.98 -3.16 H2

H2O(g) -1.43 -0.00 1.43 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.41 -3.33 -2.91 O2

Initial solution 35. 29/8/2012 20:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.825e-003 2.825e-003

Ca 1.032e-003 1.032e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.290e-004 9.290e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.830

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 293

Density (g/cm3) = 0.99648

Activity of water = 1.000

Ionic strength = 4.394e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.608e-003

Total CO2 (mol/kg) = 2.608e-003

Temperature (deg C) = 27.850

Electrical balance (eq) = 2.090e-006

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.04

Iterations = 7

Total H = 1.110148e+002

Total O = 5.551543e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.6230 0.6941

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.999e-006 8.369e-006 -5.046 -5.077 -0.032

H+ 1.579e-009 1.479e-009 -8.802 -8.830 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.608e-003

HCO3- 2.355e-003 2.196e-003 -2.628 -2.658 -0.030

CO3-2 9.734e-005 7.360e-005 -4.012 -4.133 -0.121

CaCO3 9.021e-005 9.030e-005 -4.045 -4.044 0.000

MgCO3 2.634e-005 2.637e-005 -4.579 -4.579 0.000

CaHCO3+ 2.153e-005 2.008e-005 -4.667 -4.697 -0.030

MgHCO3+ 1.006e-005 9.361e-006 -4.998 -5.029 -0.031

CO2 7.061e-006 7.068e-006 -5.151 -5.151 0.000

NaCO3- 1.577e-008 1.468e-008 -7.802 -7.833 -0.031

NaHCO3 1.146e-008 1.148e-008 -7.941 -7.940 0.000

Ca 1.032e-003

Ca+2 9.102e-004 6.878e-004 -3.041 -3.163 -0.122

CaCO3 9.021e-005 9.030e-005 -4.045 -4.044 0.000

CaHCO3+ 2.153e-005 2.008e-005 -4.667 -4.697 -0.030

CaSO4 1.043e-005 1.044e-005 -4.982 -4.981 0.000

CaOH+ 8.291e-008 7.717e-008 -7.081 -7.113 -0.031

CaHSO4+ 1.008e-013 9.382e-014 -12.997 -13.028 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.327e-005 -4.242 -4.274 -0.031

H(0) 3.009e-029

H2 1.504e-029 1.506e-029 -28.823 -28.822 0.000

K 3.325e-006

K+ 3.324e-006 3.091e-006 -5.478 -5.510 -0.031

KSO4- 1.816e-009 1.690e-009 -8.741 -8.772 -0.031

KOH 7.239e-012 7.246e-012 -11.140 -11.140 0.000

Mg 5.184e-004

Mg+2 4.741e-004 3.594e-004 -3.324 -3.444 -0.120

MgCO3 2.634e-005 2.637e-005 -4.579 -4.579 0.000

MgHCO3+ 1.006e-005 9.361e-006 -4.998 -5.029 -0.031

MgSO4 6.705e-006 6.712e-006 -5.174 -5.173 0.000

MgOH+ 1.223e-006 1.138e-006 -5.913 -5.944 -0.031

Na 1.001e-005

Na+ 9.976e-006 9.291e-006 -5.001 -5.032 -0.031

NaCO3- 1.577e-008 1.468e-008 -7.802 -7.833 -0.031

NaHCO3 1.146e-008 1.148e-008 -7.941 -7.940 0.000

NaSO4- 3.773e-009 3.512e-009 -8.423 -8.454 -0.031

NaOH 4.146e-011 4.150e-011 -10.382 -10.382 0.000

O(0) 9.290e-004

O2 4.645e-004 4.650e-004 -3.333 -3.333 0.000

S(6) 1.154e-004

SO4-2 9.823e-005 7.408e-005 -4.008 -4.130 -0.123

CaSO4 1.043e-005 1.044e-005 -4.982 -4.981 0.000

MgSO4 6.705e-006 6.712e-006 -5.174 -5.173 0.000

NaSO4- 3.773e-009 3.512e-009 -8.423 -8.454 -0.031

KSO4- 1.816e-009 1.690e-009 -8.741 -8.772 -0.031

HSO4- 1.219e-011 1.134e-011 -10.914 -10.945 -0.031

CaHSO4+ 1.008e-013 9.382e-014 -12.997 -13.028 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.92 -7.29 -4.37 CaSO4

Aragonite 1.06 -7.30 -8.35 CaCO3

Calcite 1.20 -7.30 -8.50 CaCO3

CO2(g) -3.65 -5.15 -1.50 CO2

Dolomite 2.28 -14.87 -17.16 CaMg(CO3)2

Gypsum -2.71 -7.29 -4.58 CaSO4:2H2O

H2(g) -25.66 -28.82 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.42 -3.33 -2.91 O2

Initial solution 36. 29/8/2012 20:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.845e-003 2.845e-003

Ca 1.040e-003 1.040e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.152e-004 9.152e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.730

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 296

Density (g/cm3) = 0.99653

Activity of water = 1.000

Ionic strength = 4.456e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.669e-003

Total CO2 (mol/kg) = 2.669e-003

Temperature (deg C) = 27.690

Electrical balance (eq) = -3.427e-006

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.06

Iterations = 7

Total H = 1.110149e+002

Total O = 5.551560e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.7344 0.7004

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 7.068e-006 6.570e-006 -5.151 -5.182 -0.032

H+ 1.988e-009 1.862e-009 -8.701 -8.730 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.669e-003

HCO3- 2.449e-003 2.283e-003 -2.611 -2.642 -0.031

CO3-2 8.025e-005 6.057e-005 -4.096 -4.218 -0.122

CaCO3 7.554e-005 7.562e-005 -4.122 -4.121 0.000

CaHCO3+ 2.281e-005 2.126e-005 -4.642 -4.672 -0.031

MgCO3 2.179e-005 2.181e-005 -4.662 -4.661 0.000

MgHCO3+ 1.053e-005 9.793e-006 -4.978 -5.009 -0.031

CO2 9.255e-006 9.264e-006 -5.034 -5.033 0.000

NaCO3- 1.288e-008 1.199e-008 -7.890 -7.921 -0.031

NaHCO3 1.191e-008 1.192e-008 -7.924 -7.924 0.000

Ca 1.040e-003

Ca+2 9.309e-004 7.023e-004 -3.031 -3.153 -0.122

CaCO3 7.554e-005 7.562e-005 -4.122 -4.121 0.000

CaHCO3+ 2.281e-005 2.126e-005 -4.642 -4.672 -0.031

CaSO4 1.060e-005 1.061e-005 -4.975 -4.974 0.000

CaOH+ 6.727e-008 6.259e-008 -7.172 -7.203 -0.031

CaHSO4+ 1.287e-013 1.198e-013 -12.890 -12.922 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.325e-005 -4.242 -4.274 -0.032

H(0) 4.776e-029

H2 2.388e-029 2.390e-029 -28.622 -28.622 0.000

K 3.325e-006

K+ 3.324e-006 3.090e-006 -5.478 -5.510 -0.032

KSO4- 1.805e-009 1.679e-009 -8.744 -8.775 -0.031

KOH 5.748e-012 5.754e-012 -11.241 -11.240 0.000

Mg 5.184e-004

Mg+2 4.784e-004 3.621e-004 -3.320 -3.441 -0.121

MgCO3 2.179e-005 2.181e-005 -4.662 -4.661 0.000

MgHCO3+ 1.053e-005 9.793e-006 -4.978 -5.009 -0.031

MgSO4 6.705e-006 6.712e-006 -5.174 -5.173 0.000

MgOH+ 9.652e-007 8.981e-007 -6.015 -6.047 -0.031

Na 1.001e-005

Na+ 9.978e-006 9.290e-006 -5.001 -5.032 -0.031

NaCO3- 1.288e-008 1.199e-008 -7.890 -7.921 -0.031

NaHCO3 1.191e-008 1.192e-008 -7.924 -7.924 0.000

NaSO4- 3.757e-009 3.496e-009 -8.425 -8.456 -0.031

NaOH 3.292e-011 3.296e-011 -10.482 -10.482 0.000

O(0) 9.152e-004

O2 4.576e-004 4.581e-004 -3.339 -3.339 0.000

S(6) 1.154e-004

SO4-2 9.806e-005 7.383e-005 -4.008 -4.132 -0.123

CaSO4 1.060e-005 1.061e-005 -4.975 -4.974 0.000

MgSO4 6.705e-006 6.712e-006 -5.174 -5.173 0.000

NaSO4- 3.757e-009 3.496e-009 -8.425 -8.456 -0.031

KSO4- 1.805e-009 1.679e-009 -8.744 -8.775 -0.031

HSO4- 1.524e-011 1.418e-011 -10.817 -10.848 -0.031

CaHSO4+ 1.287e-013 1.198e-013 -12.890 -12.922 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.91 -7.29 -4.37 CaSO4

Aragonite 0.98 -7.37 -8.35 CaCO3

Calcite 1.12 -7.37 -8.50 CaCO3

CO2(g) -3.53 -5.03 -1.50 CO2

Dolomite 2.12 -15.03 -17.15 CaMg(CO3)2

Gypsum -2.70 -7.29 -4.58 CaSO4:2H2O

H2(g) -25.46 -28.62 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.43 -3.34 -2.91 O2

Initial solution 37. 29/8/2012 20:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.887e-003 2.887e-003

Ca 1.055e-003 1.055e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 8.934e-004 8.934e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.710

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 298

Density (g/cm3) = 0.99657

Activity of water = 1.000

Ionic strength = 4.508e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.716e-003

Total CO2 (mol/kg) = 2.716e-003

Temperature (deg C) = 27.540

Electrical balance (eq) = -1.495e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.26

Iterations = 7

Total H = 1.110150e+002

Total O = 5.551572e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.7640 0.7018

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 6.678e-006 6.205e-006 -5.175 -5.207 -0.032

H+ 2.083e-009 1.950e-009 -8.681 -8.710 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.716e-003

HCO3- 2.498e-003 2.328e-003 -2.602 -2.633 -0.031

CO3-2 7.804e-005 5.883e-005 -4.108 -4.230 -0.123

CaCO3 7.423e-005 7.431e-005 -4.129 -4.129 0.000

CaHCO3+ 2.357e-005 2.196e-005 -4.628 -4.658 -0.031

MgCO3 2.111e-005 2.113e-005 -4.676 -4.675 0.000

MgHCO3+ 1.073e-005 9.978e-006 -4.969 -5.001 -0.031

CO2 9.899e-006 9.909e-006 -5.004 -5.004 0.000

NaCO3- 1.242e-008 1.155e-008 -7.906 -7.937 -0.031

NaHCO3 1.214e-008 1.216e-008 -7.916 -7.915 0.000

Ca 1.055e-003

Ca+2 9.463e-004 7.129e-004 -3.024 -3.147 -0.123

CaCO3 7.423e-005 7.431e-005 -4.129 -4.129 0.000

CaHCO3+ 2.357e-005 2.196e-005 -4.628 -4.658 -0.031

CaSO4 1.072e-005 1.073e-005 -4.970 -4.969 0.000

CaOH+ 6.524e-008 6.068e-008 -7.185 -7.217 -0.031

CaHSO4+ 1.361e-013 1.266e-013 -12.866 -12.898 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.323e-005 -4.242 -4.274 -0.032

H(0) 5.244e-029

H2 2.622e-029 2.625e-029 -28.581 -28.581 0.000

K 3.325e-006

K+ 3.324e-006 3.089e-006 -5.478 -5.510 -0.032

KSO4- 1.796e-009 1.671e-009 -8.746 -8.777 -0.031

KOH 5.487e-012 5.493e-012 -11.261 -11.260 0.000

Mg 5.184e-004

Mg+2 4.790e-004 3.620e-004 -3.320 -3.441 -0.122

MgCO3 2.111e-005 2.113e-005 -4.676 -4.675 0.000

MgHCO3+ 1.073e-005 9.978e-006 -4.969 -5.001 -0.031

MgSO4 6.663e-006 6.670e-006 -5.176 -5.176 0.000

MgOH+ 9.098e-007 8.462e-007 -6.041 -6.073 -0.031

Na 1.001e-005

Na+ 9.979e-006 9.286e-006 -5.001 -5.032 -0.031

NaCO3- 1.242e-008 1.155e-008 -7.906 -7.937 -0.031

NaHCO3 1.214e-008 1.216e-008 -7.916 -7.915 0.000

NaSO4- 3.746e-009 3.484e-009 -8.426 -8.458 -0.031

NaOH 3.143e-011 3.146e-011 -10.503 -10.502 0.000

O(0) 8.934e-004

O2 4.467e-004 4.471e-004 -3.350 -3.350 0.000

S(6) 1.154e-004

SO4-2 9.798e-005 7.366e-005 -4.009 -4.133 -0.124

CaSO4 1.072e-005 1.073e-005 -4.970 -4.969 0.000

MgSO4 6.663e-006 6.670e-006 -5.176 -5.176 0.000

NaSO4- 3.746e-009 3.484e-009 -8.426 -8.458 -0.031

KSO4- 1.796e-009 1.671e-009 -8.746 -8.777 -0.031

HSO4- 1.588e-011 1.477e-011 -10.799 -10.831 -0.031

CaHSO4+ 1.361e-013 1.266e-013 -12.866 -12.898 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.91 -7.28 -4.37 CaSO4

Aragonite 0.98 -7.38 -8.35 CaCO3

Calcite 1.12 -7.38 -8.49 CaCO3

CO2(g) -3.51 -5.00 -1.50 CO2

Dolomite 2.10 -15.05 -17.15 CaMg(CO3)2

Gypsum -2.70 -7.28 -4.58 CaSO4:2H2O

H2(g) -25.42 -28.58 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.44 -3.35 -2.91 O2

Initial solution 38. 29/8/2012 21:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.897e-003 2.897e-003

Ca 1.059e-003 1.059e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 8.765e-004 8.765e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.670

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 299

Density (g/cm3) = 0.99660

Activity of water = 1.000

Ionic strength = 4.534e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.741e-003

Total CO2 (mol/kg) = 2.741e-003

Temperature (deg C) = 27.430

Electrical balance (eq) = -1.779e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.30

Iterations = 8

Total H = 1.110150e+002

Total O = 5.551577e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8109 0.7044

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 6.042e-006 5.614e-006 -5.219 -5.251 -0.032

H+ 2.284e-009 2.138e-009 -8.641 -8.670 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.741e-003

HCO3- 2.534e-003 2.361e-003 -2.596 -2.627 -0.031

CO3-2 7.209e-005 5.430e-005 -4.142 -4.265 -0.123

CaCO3 6.893e-005 6.900e-005 -4.162 -4.161 0.000

CaHCO3+ 2.407e-005 2.243e-005 -4.618 -4.649 -0.031

MgCO3 1.950e-005 1.952e-005 -4.710 -4.709 0.000

CO2 1.102e-005 1.103e-005 -4.958 -4.957 0.000

MgHCO3+ 1.091e-005 1.014e-005 -4.962 -4.994 -0.032

NaHCO3 1.232e-008 1.233e-008 -7.910 -7.909 0.000

NaCO3- 1.140e-008 1.060e-008 -7.943 -7.975 -0.032

Ca 1.059e-003

Ca+2 9.548e-004 7.189e-004 -3.020 -3.143 -0.123

CaCO3 6.893e-005 6.900e-005 -4.162 -4.161 0.000

CaHCO3+ 2.407e-005 2.243e-005 -4.618 -4.649 -0.031

CaSO4 1.078e-005 1.079e-005 -4.967 -4.967 0.000

CaOH+ 6.000e-008 5.580e-008 -7.222 -7.253 -0.032

CaHSO4+ 1.499e-013 1.394e-013 -12.824 -12.856 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.322e-005 -4.242 -4.274 -0.032

H(0) 6.312e-029

H2 3.156e-029 3.159e-029 -28.501 -28.500 0.000

K 3.326e-006

K+ 3.324e-006 3.088e-006 -5.478 -5.510 -0.032

KSO4- 1.791e-009 1.665e-009 -8.747 -8.779 -0.032

KOH 5.003e-012 5.008e-012 -11.301 -11.300 0.000

Mg 5.184e-004

Mg+2 4.805e-004 3.629e-004 -3.318 -3.440 -0.122

MgCO3 1.950e-005 1.952e-005 -4.710 -4.709 0.000

MgHCO3+ 1.091e-005 1.014e-005 -4.962 -4.994 -0.032

MgSO4 6.653e-006 6.660e-006 -5.177 -5.177 0.000

MgOH+ 8.239e-007 7.661e-007 -6.084 -6.116 -0.032

Na 1.001e-005

Na+ 9.980e-006 9.286e-006 -5.001 -5.032 -0.031

NaHCO3 1.232e-008 1.233e-008 -7.910 -7.909 0.000

NaCO3- 1.140e-008 1.060e-008 -7.943 -7.975 -0.032

NaSO4- 3.739e-009 3.477e-009 -8.427 -8.459 -0.032

NaOH 2.866e-011 2.869e-011 -10.543 -10.542 0.000

O(0) 8.765e-004

O2 4.382e-004 4.387e-004 -3.358 -3.358 0.000

S(6) 1.154e-004

SO4-2 9.793e-005 7.357e-005 -4.009 -4.133 -0.124

CaSO4 1.078e-005 1.079e-005 -4.967 -4.967 0.000

MgSO4 6.653e-006 6.660e-006 -5.177 -5.177 0.000

NaSO4- 3.739e-009 3.477e-009 -8.427 -8.459 -0.032

KSO4- 1.791e-009 1.665e-009 -8.747 -8.779 -0.032

HSO4- 1.735e-011 1.613e-011 -10.761 -10.792 -0.032

CaHSO4+ 1.499e-013 1.394e-013 -12.824 -12.856 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.90 -7.28 -4.37 CaSO4

Aragonite 0.94 -7.41 -8.35 CaCO3

Calcite 1.09 -7.41 -8.49 CaCO3

CO2(g) -3.46 -4.96 -1.50 CO2

Dolomite 2.03 -15.11 -17.15 CaMg(CO3)2

Gypsum -2.69 -7.28 -4.58 CaSO4:2H2O

H2(g) -25.34 -28.50 -3.16 H2

H2O(g) -1.45 -0.00 1.45 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.45 -3.36 -2.91 O2

Initial solution 39. 29/8/2012 21:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.907e-003 2.907e-003

Ca 1.062e-003 1.062e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 8.571e-004 8.571e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.610

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 301

Density (g/cm3) = 0.99664

Activity of water = 1.000

Ionic strength = 4.566e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.772e-003

Total CO2 (mol/kg) = 2.772e-003

Temperature (deg C) = 27.300

Electrical balance (eq) = -2.047e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.35

Iterations = 8

Total H = 1.110151e+002

Total O = 5.551584e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8791 0.7081

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 5.214e-006 4.843e-006 -5.283 -5.315 -0.032

H+ 2.623e-009 2.455e-009 -8.581 -8.610 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.772e-003

HCO3- 2.581e-003 2.404e-003 -2.588 -2.619 -0.031

CO3-2 6.382e-005 4.803e-005 -4.195 -4.318 -0.123

CaCO3 6.141e-005 6.148e-005 -4.212 -4.211 0.000

CaHCO3+ 2.472e-005 2.302e-005 -4.607 -4.638 -0.031

MgCO3 1.728e-005 1.729e-005 -4.763 -4.762 0.000

CO2 1.290e-005 1.292e-005 -4.889 -4.889 0.000

MgHCO3+ 1.114e-005 1.035e-005 -4.953 -4.985 -0.032

NaHCO3 1.254e-008 1.255e-008 -7.902 -7.901 0.000

NaCO3- 1.002e-008 9.318e-009 -7.999 -8.031 -0.032

Ca 1.062e-003

Ca+2 9.654e-004 7.262e-004 -3.015 -3.139 -0.124

CaCO3 6.141e-005 6.148e-005 -4.212 -4.211 0.000

CaHCO3+ 2.472e-005 2.302e-005 -4.607 -4.638 -0.031

CaSO4 1.086e-005 1.087e-005 -4.964 -4.964 0.000

CaOH+ 5.281e-008 4.909e-008 -7.277 -7.309 -0.032

CaHSO4+ 1.732e-013 1.610e-013 -12.761 -12.793 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.321e-005 -4.242 -4.274 -0.032

H(0) 8.331e-029

H2 4.166e-029 4.170e-029 -28.380 -28.380 0.000

K 3.326e-006

K+ 3.324e-006 3.088e-006 -5.478 -5.510 -0.032

KSO4- 1.784e-009 1.658e-009 -8.749 -8.780 -0.032

KOH 4.357e-012 4.361e-012 -11.361 -11.360 0.000

Mg 5.184e-004

Mg+2 4.826e-004 3.642e-004 -3.316 -3.439 -0.122

MgCO3 1.728e-005 1.729e-005 -4.763 -4.762 0.000

MgHCO3+ 1.114e-005 1.035e-005 -4.953 -4.985 -0.032

MgSO4 6.645e-006 6.652e-006 -5.178 -5.177 0.000

MgOH+ 7.120e-007 6.620e-007 -6.147 -6.179 -0.032

Na 1.001e-005

Na+ 9.981e-006 9.285e-006 -5.001 -5.032 -0.031

NaHCO3 1.254e-008 1.255e-008 -7.902 -7.901 0.000

NaCO3- 1.002e-008 9.318e-009 -7.999 -8.031 -0.032

NaSO4- 3.730e-009 3.468e-009 -8.428 -8.460 -0.032

NaOH 2.496e-011 2.499e-011 -10.603 -10.602 0.000

O(0) 8.571e-004

O2 4.285e-004 4.290e-004 -3.368 -3.368 0.000

S(6) 1.154e-004

SO4-2 9.786e-005 7.346e-005 -4.009 -4.134 -0.125

CaSO4 1.086e-005 1.087e-005 -4.964 -4.964 0.000

MgSO4 6.645e-006 6.652e-006 -5.178 -5.177 0.000

NaSO4- 3.730e-009 3.468e-009 -8.428 -8.460 -0.032

KSO4- 1.784e-009 1.658e-009 -8.749 -8.780 -0.032

HSO4- 1.984e-011 1.844e-011 -10.703 -10.734 -0.032

CaHSO4+ 1.732e-013 1.610e-013 -12.761 -12.793 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.90 -7.27 -4.37 CaSO4

Aragonite 0.89 -7.46 -8.35 CaCO3

Calcite 1.04 -7.46 -8.49 CaCO3

CO2(g) -3.39 -4.89 -1.49 CO2

Dolomite 1.93 -15.21 -17.14 CaMg(CO3)2

Gypsum -2.69 -7.27 -4.58 CaSO4:2H2O

H2(g) -25.22 -28.38 -3.16 H2

H2O(g) -1.45 -0.00 1.45 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.46 -3.37 -2.91 O2

Initial solution 40. 29/8/2012 21:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.918e-003 2.918e-003

Ca 1.066e-003 1.066e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 8.358e-004 8.358e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.560

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 302

Density (g/cm3) = 0.99666

Activity of water = 1.000

Ionic strength = 4.593e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.798e-003

Total CO2 (mol/kg) = 2.798e-003

Temperature (deg C) = 27.220

Electrical balance (eq) = -2.347e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.39

Iterations = 8

Total H = 1.110151e+002

Total O = 5.551590e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9329 0.7112

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 4.620e-006 4.291e-006 -5.335 -5.367 -0.032

H+ 2.943e-009 2.754e-009 -8.531 -8.560 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.798e-003

HCO3- 2.618e-003 2.438e-003 -2.582 -2.613 -0.031

CO3-2 5.764e-005 4.336e-005 -4.239 -4.363 -0.124

CaCO3 5.580e-005 5.586e-005 -4.253 -4.253 0.000

CaHCO3+ 2.526e-005 2.352e-005 -4.598 -4.629 -0.031

MgCO3 1.561e-005 1.563e-005 -4.806 -4.806 0.000

CO2 1.470e-005 1.471e-005 -4.833 -4.832 0.000

MgHCO3+ 1.132e-005 1.052e-005 -4.946 -4.978 -0.032

NaHCO3 1.271e-008 1.273e-008 -7.896 -7.895 0.000

NaCO3- 9.011e-009 8.376e-009 -8.045 -8.077 -0.032

Ca 1.066e-003

Ca+2 9.741e-004 7.323e-004 -3.011 -3.135 -0.124

CaCO3 5.580e-005 5.586e-005 -4.253 -4.253 0.000

CaHCO3+ 2.526e-005 2.352e-005 -4.598 -4.629 -0.031

CaSO4 1.093e-005 1.094e-005 -4.961 -4.961 0.000

CaOH+ 4.746e-008 4.412e-008 -7.324 -7.355 -0.032

CaHSO4+ 1.954e-013 1.816e-013 -12.709 -12.741 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.320e-005 -4.242 -4.274 -0.032

H(0) 1.050e-028

H2 5.248e-029 5.254e-029 -28.280 -28.280 0.000

K 3.326e-006

K+ 3.324e-006 3.087e-006 -5.478 -5.510 -0.032

KSO4- 1.779e-009 1.654e-009 -8.750 -8.782 -0.032

KOH 3.882e-012 3.886e-012 -11.411 -11.410 0.000

Mg 5.184e-004

Mg+2 4.842e-004 3.651e-004 -3.315 -3.438 -0.123

MgCO3 1.561e-005 1.563e-005 -4.806 -4.806 0.000

MgHCO3+ 1.132e-005 1.052e-005 -4.946 -4.978 -0.032

MgSO4 6.639e-006 6.646e-006 -5.178 -5.177 0.000

MgOH+ 6.318e-007 5.873e-007 -6.199 -6.231 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.284e-006 -5.001 -5.032 -0.031

NaHCO3 1.271e-008 1.273e-008 -7.896 -7.895 0.000

NaCO3- 9.011e-009 8.376e-009 -8.045 -8.077 -0.032

NaSO4- 3.724e-009 3.461e-009 -8.429 -8.461 -0.032

NaOH 2.225e-011 2.227e-011 -10.653 -10.652 0.000

O(0) 8.358e-004

O2 4.179e-004 4.184e-004 -3.379 -3.378 0.000

S(6) 1.154e-004

SO4-2 9.780e-005 7.336e-005 -4.010 -4.135 -0.125

CaSO4 1.093e-005 1.094e-005 -4.961 -4.961 0.000

MgSO4 6.639e-006 6.646e-006 -5.178 -5.177 0.000

NaSO4- 3.724e-009 3.461e-009 -8.429 -8.461 -0.032

KSO4- 1.779e-009 1.654e-009 -8.750 -8.782 -0.032

HSO4- 2.219e-011 2.063e-011 -10.654 -10.686 -0.032

CaHSO4+ 1.954e-013 1.816e-013 -12.709 -12.741 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.90 -7.27 -4.37 CaSO4

Aragonite 0.85 -7.50 -8.35 CaCO3

Calcite 0.99 -7.50 -8.49 CaCO3

CO2(g) -3.34 -4.83 -1.49 CO2

Dolomite 1.84 -15.30 -17.14 CaMg(CO3)2

Gypsum -2.69 -7.27 -4.58 CaSO4:2H2O

H2(g) -25.12 -28.28 -3.16 H2

H2O(g) -1.45 -0.00 1.45 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.47 -3.38 -2.91 O2

Initial solution 41. 29/8/2012 21:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.938e-003 2.938e-003

Ca 1.074e-003 1.074e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 8.177e-004 8.177e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.490

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 304

Density (g/cm3) = 0.99670

Activity of water = 1.000

Ionic strength = 4.635e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.839e-003

Total CO2 (mol/kg) = 2.839e-003

Temperature (deg C) = 27.100

Electrical balance (eq) = -2.899e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.48

Iterations = 8

Total H = 1.110151e+002

Total O = 5.551600e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.0103 0.7155

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.899e-006 3.620e-006 -5.409 -5.441 -0.032

H+ 3.459e-009 3.236e-009 -8.461 -8.490 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.839e-003

HCO3- 2.671e-003 2.487e-003 -2.573 -2.604 -0.031

CO3-2 5.000e-005 3.756e-005 -4.301 -4.425 -0.124

CaCO3 4.883e-005 4.888e-005 -4.311 -4.311 0.000

CaHCO3+ 2.606e-005 2.426e-005 -4.584 -4.615 -0.031

CO2 1.764e-005 1.766e-005 -4.754 -4.753 0.000

MgCO3 1.354e-005 1.356e-005 -4.868 -4.868 0.000

MgHCO3+ 1.158e-005 1.076e-005 -4.936 -4.968 -0.032

NaHCO3 1.297e-008 1.298e-008 -7.887 -7.887 0.000

NaCO3- 7.761e-009 7.212e-009 -8.110 -8.142 -0.032

Ca 1.074e-003

Ca+2 9.877e-004 7.416e-004 -3.005 -3.130 -0.124

CaCO3 4.883e-005 4.888e-005 -4.311 -4.311 0.000

CaHCO3+ 2.606e-005 2.426e-005 -4.584 -4.615 -0.031

CaSO4 1.103e-005 1.105e-005 -4.957 -4.957 0.000

CaOH+ 4.093e-008 3.803e-008 -7.388 -7.420 -0.032

CaHSO4+ 2.314e-013 2.151e-013 -12.636 -12.667 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.318e-005 -4.242 -4.274 -0.032

H(0) 1.451e-028

H2 7.253e-029 7.261e-029 -28.139 -28.139 0.000

K 3.326e-006

K+ 3.324e-006 3.086e-006 -5.478 -5.511 -0.032

KSO4- 1.772e-009 1.646e-009 -8.752 -8.783 -0.032

KOH 3.303e-012 3.307e-012 -11.481 -11.481 0.000

Mg 5.184e-004

Mg+2 4.861e-004 3.662e-004 -3.313 -3.436 -0.123

MgCO3 1.354e-005 1.356e-005 -4.868 -4.868 0.000

MgHCO3+ 1.158e-005 1.076e-005 -4.936 -4.968 -0.032

MgSO4 6.624e-006 6.631e-006 -5.179 -5.178 0.000

MgOH+ 5.337e-007 4.960e-007 -6.273 -6.305 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.282e-006 -5.001 -5.032 -0.032

NaHCO3 1.297e-008 1.298e-008 -7.887 -7.887 0.000

NaCO3- 7.761e-009 7.212e-009 -8.110 -8.142 -0.032

NaSO4- 3.714e-009 3.451e-009 -8.430 -8.462 -0.032

NaOH 1.893e-011 1.895e-011 -10.723 -10.722 0.000

O(0) 8.177e-004

O2 4.089e-004 4.093e-004 -3.388 -3.388 0.000

S(6) 1.154e-004

SO4-2 9.771e-005 7.321e-005 -4.010 -4.135 -0.125

CaSO4 1.103e-005 1.105e-005 -4.957 -4.957 0.000

MgSO4 6.624e-006 6.631e-006 -5.179 -5.178 0.000

NaSO4- 3.714e-009 3.451e-009 -8.430 -8.462 -0.032

KSO4- 1.772e-009 1.646e-009 -8.752 -8.783 -0.032

HSO4- 2.596e-011 2.412e-011 -10.586 -10.618 -0.032

CaHSO4+ 2.314e-013 2.151e-013 -12.636 -12.667 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.27 -4.37 CaSO4

Aragonite 0.79 -7.56 -8.35 CaCO3

Calcite 0.94 -7.56 -8.49 CaCO3

CO2(g) -3.26 -4.75 -1.49 CO2

Dolomite 1.72 -15.42 -17.14 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.98 -28.14 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.48 -3.39 -2.91 O2

Initial solution 42. 29/8/2012 22:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 7.933e-004 7.933e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.430

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 306

Density (g/cm3) = 0.99673

Activity of water = 1.000

Ionic strength = 4.673e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.876e-003

Total CO2 (mol/kg) = 2.876e-003

Temperature (deg C) = 26.990

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551608e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.0760 0.7191

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.369e-006 3.127e-006 -5.472 -5.505 -0.032

H+ 3.972e-009 3.715e-009 -8.401 -8.430 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.876e-003

HCO3- 2.717e-003 2.529e-003 -2.566 -2.597 -0.031

CO3-2 4.423e-005 3.320e-005 -4.354 -4.479 -0.125

CaCO3 4.354e-005 4.358e-005 -4.361 -4.361 0.000

CaHCO3+ 2.676e-005 2.491e-005 -4.572 -4.604 -0.031

CO2 2.062e-005 2.064e-005 -4.686 -4.685 0.000

MgCO3 1.197e-005 1.198e-005 -4.922 -4.921 0.000

MgHCO3+ 1.180e-005 1.096e-005 -4.928 -4.960 -0.032

NaHCO3 1.318e-008 1.320e-008 -7.880 -7.879 0.000

NaCO3- 6.823e-009 6.338e-009 -8.166 -8.198 -0.032

Ca 1.081e-003

Ca+2 9.997e-004 7.499e-004 -3.000 -3.125 -0.125

CaCO3 4.354e-005 4.358e-005 -4.361 -4.361 0.000

CaHCO3+ 2.676e-005 2.491e-005 -4.572 -4.604 -0.031

CaSO4 1.113e-005 1.114e-005 -4.954 -4.953 0.000

CaOH+ 3.605e-008 3.349e-008 -7.443 -7.475 -0.032

CaHSO4+ 2.676e-013 2.486e-013 -12.572 -12.604 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.317e-005 -4.242 -4.274 -0.032

H(0) 1.914e-028

H2 9.572e-029 9.582e-029 -28.019 -28.019 0.000

K 3.326e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.765e-009 1.640e-009 -8.753 -8.785 -0.032

KOH 2.876e-012 2.879e-012 -11.541 -11.541 0.000

Mg 5.184e-004

Mg+2 4.876e-004 3.669e-004 -3.312 -3.435 -0.123

MgCO3 1.197e-005 1.198e-005 -4.922 -4.921 0.000

MgHCO3+ 1.180e-005 1.096e-005 -4.928 -4.960 -0.032

MgSO4 6.607e-006 6.614e-006 -5.180 -5.180 0.000

MgOH+ 4.614e-007 4.286e-007 -6.336 -6.368 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.280e-006 -5.001 -5.032 -0.032

NaHCO3 1.318e-008 1.320e-008 -7.880 -7.879 0.000

NaCO3- 6.823e-009 6.338e-009 -8.166 -8.198 -0.032

NaSO4- 3.705e-009 3.442e-009 -8.431 -8.463 -0.032

NaOH 1.648e-011 1.650e-011 -10.783 -10.782 0.000

O(0) 7.933e-004

O2 3.967e-004 3.971e-004 -3.402 -3.401 0.000

S(6) 1.154e-004

SO4-2 9.763e-005 7.308e-005 -4.010 -4.136 -0.126

CaSO4 1.113e-005 1.114e-005 -4.954 -4.953 0.000

MgSO4 6.607e-006 6.614e-006 -5.180 -5.180 0.000

NaSO4- 3.705e-009 3.442e-009 -8.431 -8.463 -0.032

KSO4- 1.765e-009 1.640e-009 -8.753 -8.785 -0.032

HSO4- 2.969e-011 2.758e-011 -10.527 -10.559 -0.032

CaHSO4+ 2.676e-013 2.486e-013 -12.572 -12.604 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.26 -4.37 CaSO4

Aragonite 0.75 -7.60 -8.35 CaCO3

Calcite 0.89 -7.60 -8.49 CaCO3

CO2(g) -3.19 -4.69 -1.49 CO2

Dolomite 1.62 -15.52 -17.14 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.86 -28.02 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.49 -3.40 -2.91 O2

Initial solution 43. 29/8/2012 22:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.980e-003 2.980e-003

Ca 1.089e-003 1.089e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 7.602e-004 7.602e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.350

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 308

Density (g/cm3) = 0.99676

Activity of water = 1.000

Ionic strength = 4.714e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.917e-003

Total CO2 (mol/kg) = 2.917e-003

Temperature (deg C) = 26.880

Electrical balance (eq) = -4.035e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.66

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551617e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1603 0.7239

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.780e-006 2.580e-006 -5.556 -5.588 -0.033

H+ 4.777e-009 4.467e-009 -8.321 -8.350 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.917e-003

HCO3- 2.768e-003 2.575e-003 -2.558 -2.589 -0.031

CO3-2 3.742e-005 2.806e-005 -4.427 -4.552 -0.125

CaCO3 3.714e-005 3.719e-005 -4.430 -4.430 0.000

CaHCO3+ 2.754e-005 2.563e-005 -4.560 -4.591 -0.031

CO2 2.527e-005 2.530e-005 -4.597 -4.597 0.000

MgHCO3+ 1.204e-005 1.118e-005 -4.919 -4.952 -0.032

MgCO3 1.013e-005 1.014e-005 -4.995 -4.994 0.000

NaHCO3 1.342e-008 1.344e-008 -7.872 -7.872 0.000

NaCO3- 5.735e-009 5.326e-009 -8.241 -8.274 -0.032

Ca 1.089e-003

Ca+2 1.013e-003 7.588e-004 -2.995 -3.120 -0.125

CaCO3 3.714e-005 3.719e-005 -4.430 -4.430 0.000

CaHCO3+ 2.754e-005 2.563e-005 -4.560 -4.591 -0.031

CaSO4 1.122e-005 1.124e-005 -4.950 -4.949 0.000

CaOH+ 3.035e-008 2.819e-008 -7.518 -7.550 -0.032

CaHSO4+ 3.243e-013 3.012e-013 -12.489 -12.521 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.274 -0.032

H(0) 2.770e-028

H2 1.385e-028 1.387e-028 -27.859 -27.858 0.000

K 3.326e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.758e-009 1.633e-009 -8.755 -8.787 -0.032

KOH 2.392e-012 2.394e-012 -11.621 -11.621 0.000

Mg 5.184e-004

Mg+2 4.893e-004 3.678e-004 -3.310 -3.434 -0.124

MgHCO3+ 1.204e-005 1.118e-005 -4.919 -4.952 -0.032

MgCO3 1.013e-005 1.014e-005 -4.995 -4.994 0.000

MgSO4 6.592e-006 6.599e-006 -5.181 -5.181 0.000

MgOH+ 3.811e-007 3.539e-007 -6.419 -6.451 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.279e-006 -5.001 -5.033 -0.032

NaHCO3 1.342e-008 1.344e-008 -7.872 -7.872 0.000

NaCO3- 5.735e-009 5.326e-009 -8.241 -8.274 -0.032

NaSO4- 3.695e-009 3.432e-009 -8.432 -8.464 -0.032

NaOH 1.371e-011 1.372e-011 -10.863 -10.863 0.000

O(0) 7.602e-004

O2 3.801e-004 3.805e-004 -3.420 -3.420 0.000

S(6) 1.154e-004

SO4-2 9.755e-005 7.293e-005 -4.011 -4.137 -0.126

CaSO4 1.122e-005 1.124e-005 -4.950 -4.949 0.000

MgSO4 6.592e-006 6.599e-006 -5.181 -5.181 0.000

NaSO4- 3.695e-009 3.432e-009 -8.432 -8.464 -0.032

KSO4- 1.758e-009 1.633e-009 -8.755 -8.787 -0.032

HSO4- 3.554e-011 3.301e-011 -10.449 -10.481 -0.032

CaHSO4+ 3.243e-013 3.012e-013 -12.489 -12.521 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.26 -4.37 CaSO4

Aragonite 0.68 -7.67 -8.35 CaCO3

Calcite 0.82 -7.67 -8.49 CaCO3

CO2(g) -3.11 -4.60 -1.49 CO2

Dolomite 1.48 -15.66 -17.13 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.70 -27.86 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.51 -3.42 -2.91 O2

Initial solution 44. 29/8/2012 22:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.990e-003 2.990e-003

Ca 1.092e-003 1.092e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 7.421e-004 7.421e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.250

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 309

Density (g/cm3) = 0.99679

Activity of water = 1.000

Ionic strength = 4.745e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.952e-003

Total CO2 (mol/kg) = 2.952e-003

Temperature (deg C) = 26.760

Electrical balance (eq) = -4.336e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.70

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551625e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.2675 0.7300

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.189e-006 2.031e-006 -5.660 -5.692 -0.033

H+ 6.015e-009 5.623e-009 -8.221 -8.250 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.952e-003

HCO3- 2.810e-003 2.615e-003 -2.551 -2.583 -0.031

CO2 3.235e-005 3.238e-005 -4.490 -4.490 0.000

CO3-2 3.013e-005 2.257e-005 -4.521 -4.646 -0.125

CaCO3 3.009e-005 3.012e-005 -4.522 -4.521 0.000

CaHCO3+ 2.818e-005 2.622e-005 -4.550 -4.581 -0.031

MgHCO3+ 1.226e-005 1.138e-005 -4.912 -4.944 -0.032

MgCO3 8.156e-006 8.165e-006 -5.088 -5.088 0.000

NaHCO3 1.363e-008 1.364e-008 -7.866 -7.865 0.000

NaCO3- 4.588e-009 4.260e-009 -8.338 -8.371 -0.032

Ca 1.092e-003

Ca+2 1.023e-003 7.658e-004 -2.990 -3.116 -0.126

CaCO3 3.009e-005 3.012e-005 -4.522 -4.521 0.000

CaHCO3+ 2.818e-005 2.622e-005 -4.550 -4.581 -0.031

CaSO4 1.130e-005 1.131e-005 -4.947 -4.946 0.000

CaOH+ 2.434e-008 2.260e-008 -7.614 -7.646 -0.032

CaHSO4+ 4.104e-013 3.811e-013 -12.387 -12.419 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 4.395e-028

H2 2.198e-028 2.200e-028 -27.658 -27.658 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.752e-009 1.627e-009 -8.756 -8.789 -0.032

KOH 1.899e-012 1.901e-012 -11.721 -11.721 0.000

Mg 5.184e-004

Mg+2 4.911e-004 3.689e-004 -3.309 -3.433 -0.124

MgHCO3+ 1.226e-005 1.138e-005 -4.912 -4.944 -0.032

MgCO3 8.156e-006 8.165e-006 -5.088 -5.088 0.000

MgSO4 6.582e-006 6.589e-006 -5.182 -5.181 0.000

MgOH+ 3.004e-007 2.790e-007 -6.522 -6.554 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.278e-006 -5.001 -5.033 -0.032

NaHCO3 1.363e-008 1.364e-008 -7.866 -7.865 0.000

NaCO3- 4.588e-009 4.260e-009 -8.338 -8.371 -0.032

NaSO4- 3.688e-009 3.424e-009 -8.433 -8.465 -0.032

NaOH 1.089e-011 1.090e-011 -10.963 -10.963 0.000

O(0) 7.421e-004

O2 3.710e-004 3.714e-004 -3.431 -3.430 0.000

S(6) 1.154e-004

SO4-2 9.748e-005 7.283e-005 -4.011 -4.138 -0.127

CaSO4 1.130e-005 1.131e-005 -4.947 -4.946 0.000

MgSO4 6.582e-006 6.589e-006 -5.182 -5.181 0.000

NaSO4- 3.688e-009 3.424e-009 -8.433 -8.465 -0.032

KSO4- 1.752e-009 1.627e-009 -8.756 -8.789 -0.032

HSO4- 4.457e-011 4.139e-011 -10.351 -10.383 -0.032

CaHSO4+ 4.104e-013 3.811e-013 -12.387 -12.419 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.59 -7.76 -8.35 CaCO3

Calcite 0.73 -7.76 -8.49 CaCO3

CO2(g) -3.00 -4.49 -1.49 CO2

Dolomite 1.29 -15.84 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.50 -27.66 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.53 -3.43 -2.90 O2

Initial solution 45. 29/8/2012 22:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.990e-003 2.990e-003

Ca 1.092e-003 1.092e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 7.183e-004 7.183e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.190

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 309

Density (g/cm3) = 0.99682

Activity of water = 1.000

Ionic strength = 4.755e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.966e-003

Total CO2 (mol/kg) = 2.966e-003

Temperature (deg C) = 26.650

Electrical balance (eq) = -4.336e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.70

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551626e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3330 0.7336

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.891e-006 1.755e-006 -5.723 -5.756 -0.033

H+ 6.906e-009 6.457e-009 -8.161 -8.190 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.966e-003

HCO3- 2.828e-003 2.631e-003 -2.549 -2.580 -0.031

CO2 3.741e-005 3.745e-005 -4.427 -4.427 0.000

CaHCO3+ 2.840e-005 2.642e-005 -4.547 -4.578 -0.031

CO3-2 2.635e-005 1.974e-005 -4.579 -4.705 -0.126

CaCO3 2.633e-005 2.636e-005 -4.580 -4.579 0.000

MgHCO3+ 1.235e-005 1.146e-005 -4.908 -4.941 -0.032

MgCO3 7.132e-006 7.140e-006 -5.147 -5.146 0.000

NaHCO3 1.371e-008 1.372e-008 -7.863 -7.863 0.000

NaCO3- 3.990e-009 3.704e-009 -8.399 -8.431 -0.032

Ca 1.092e-003

Ca+2 1.026e-003 7.683e-004 -2.989 -3.114 -0.126

CaHCO3+ 2.840e-005 2.642e-005 -4.547 -4.578 -0.031

CaCO3 2.633e-005 2.636e-005 -4.580 -4.579 0.000

CaSO4 1.132e-005 1.133e-005 -4.946 -4.946 0.000

CaOH+ 2.127e-008 1.975e-008 -7.672 -7.705 -0.032

CaHSO4+ 4.714e-013 4.377e-013 -12.327 -12.359 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 5.800e-028

H2 2.900e-028 2.903e-028 -27.538 -27.537 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.748e-009 1.623e-009 -8.757 -8.790 -0.032

KOH 1.654e-012 1.656e-012 -11.781 -11.781 0.000

Mg 5.184e-004

Mg+2 4.921e-004 3.696e-004 -3.308 -3.432 -0.124

MgHCO3+ 1.235e-005 1.146e-005 -4.908 -4.941 -0.032

MgCO3 7.132e-006 7.140e-006 -5.147 -5.146 0.000

MgSO4 6.573e-006 6.580e-006 -5.182 -5.182 0.000

MgOH+ 2.596e-007 2.410e-007 -6.586 -6.618 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.278e-006 -5.001 -5.033 -0.032

NaHCO3 1.371e-008 1.372e-008 -7.863 -7.863 0.000

NaCO3- 3.990e-009 3.704e-009 -8.399 -8.431 -0.032

NaSO4- 3.684e-009 3.421e-009 -8.434 -8.466 -0.032

NaOH 9.483e-012 9.493e-012 -11.023 -11.023 0.000

O(0) 7.183e-004

O2 3.592e-004 3.596e-004 -3.445 -3.444 0.000

S(6) 1.154e-004

SO4-2 9.747e-005 7.280e-005 -4.011 -4.138 -0.127

CaSO4 1.132e-005 1.133e-005 -4.946 -4.946 0.000

MgSO4 6.573e-006 6.580e-006 -5.182 -5.182 0.000

NaSO4- 3.684e-009 3.421e-009 -8.434 -8.466 -0.032

KSO4- 1.748e-009 1.623e-009 -8.757 -8.790 -0.032

HSO4- 5.104e-011 4.739e-011 -10.292 -10.324 -0.032

CaHSO4+ 4.714e-013 4.377e-013 -12.327 -12.359 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.53 -7.82 -8.35 CaCO3

Calcite 0.67 -7.82 -8.49 CaCO3

CO2(g) -2.94 -4.43 -1.49 CO2

Dolomite 1.17 -15.96 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.38 -27.54 -3.16 H2

H2O(g) -1.47 -0.00 1.47 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.54 -3.44 -2.90 O2

Initial solution 46. 29/8/2012 23:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.939e-004 6.939e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.130

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 310

Density (g/cm3) = 0.99685

Activity of water = 1.000

Ionic strength = 4.787e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.000e-003

Total CO2 (mol/kg) = 3.000e-003

Temperature (deg C) = 26.550

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 7

Total H = 1.110153e+002

Total O = 5.551633e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3975 0.7372

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.636e-006 1.517e-006 -5.786 -5.819 -0.033

H+ 7.931e-009 7.413e-009 -8.101 -8.130 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.000e-003

HCO3- 2.862e-003 2.662e-003 -2.543 -2.575 -0.031

CO2 4.351e-005 4.356e-005 -4.361 -4.361 0.000

CaHCO3+ 2.895e-005 2.693e-005 -4.538 -4.570 -0.031

CaCO3 2.331e-005 2.334e-005 -4.632 -4.632 0.000

CO3-2 2.320e-005 1.736e-005 -4.635 -4.760 -0.126

MgHCO3+ 1.250e-005 1.160e-005 -4.903 -4.935 -0.032

MgCO3 6.269e-006 6.276e-006 -5.203 -5.202 0.000

NaHCO3 1.387e-008 1.388e-008 -7.858 -7.857 0.000

NaCO3- 3.492e-009 3.242e-009 -8.457 -8.489 -0.032

Ca 1.100e-003

Ca+2 1.036e-003 7.750e-004 -2.985 -3.111 -0.126

CaHCO3+ 2.895e-005 2.693e-005 -4.538 -4.570 -0.031

CaCO3 2.331e-005 2.334e-005 -4.632 -4.632 0.000

CaSO4 1.139e-005 1.141e-005 -4.943 -4.943 0.000

CaOH+ 1.869e-008 1.735e-008 -7.728 -7.761 -0.032

CaHSO4+ 5.442e-013 5.052e-013 -12.264 -12.297 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 7.654e-028

H2 3.827e-028 3.831e-028 -27.417 -27.417 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.743e-009 1.618e-009 -8.759 -8.791 -0.032

KOH 1.440e-012 1.442e-012 -11.842 -11.841 0.000

Mg 5.184e-004

Mg+2 4.929e-004 3.699e-004 -3.307 -3.432 -0.125

MgHCO3+ 1.250e-005 1.160e-005 -4.903 -4.935 -0.032

MgSO4 6.552e-006 6.559e-006 -5.184 -5.183 0.000

MgCO3 6.269e-006 6.276e-006 -5.203 -5.202 0.000

MgOH+ 2.243e-007 2.082e-007 -6.649 -6.682 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.387e-008 1.388e-008 -7.858 -7.857 0.000

NaSO4- 3.677e-009 3.413e-009 -8.435 -8.467 -0.032

NaCO3- 3.492e-009 3.242e-009 -8.457 -8.489 -0.032

NaOH 8.258e-012 8.267e-012 -11.083 -11.083 0.000

O(0) 6.939e-004

O2 3.470e-004 3.473e-004 -3.460 -3.459 0.000

S(6) 1.154e-004

SO4-2 9.742e-005 7.270e-005 -4.011 -4.138 -0.127

CaSO4 1.139e-005 1.141e-005 -4.943 -4.943 0.000

MgSO4 6.552e-006 6.559e-006 -5.184 -5.183 0.000

NaSO4- 3.677e-009 3.413e-009 -8.435 -8.467 -0.032

KSO4- 1.743e-009 1.618e-009 -8.759 -8.791 -0.032

HSO4- 5.840e-011 5.421e-011 -10.234 -10.266 -0.032

CaHSO4+ 5.442e-013 5.052e-013 -12.264 -12.297 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.48 -7.87 -8.35 CaCO3

Calcite 0.62 -7.87 -8.49 CaCO3

CO2(g) -2.88 -4.36 -1.49 CO2

Dolomite 1.06 -16.06 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.26 -27.42 -3.16 H2

H2O(g) -1.47 -0.00 1.47 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.56 -3.46 -2.90 O2

Initial solution 47. 29/8/2012 23:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.021e-003 3.021e-003

Ca 1.104e-003 1.104e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.683e-004 6.683e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.090

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 311

Density (g/cm3) = 0.99688

Activity of water = 1.000

Ionic strength = 4.804e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.019e-003

Total CO2 (mol/kg) = 3.019e-003

Temperature (deg C) = 26.450

Electrical balance (eq) = -5.188e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.82

Iterations = 7

Total H = 1.110154e+002

Total O = 5.551636e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.4416 0.7396

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.481e-006 1.373e-006 -5.830 -5.862 -0.033

H+ 8.697e-009 8.128e-009 -8.061 -8.090 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.019e-003

HCO3- 2.881e-003 2.679e-003 -2.540 -2.572 -0.032

CO2 4.808e-005 4.813e-005 -4.318 -4.318 0.000

CaHCO3+ 2.924e-005 2.719e-005 -4.534 -4.566 -0.032

CaCO3 2.142e-005 2.144e-005 -4.669 -4.669 0.000

CO3-2 2.126e-005 1.591e-005 -4.672 -4.798 -0.126

MgHCO3+ 1.258e-005 1.168e-005 -4.900 -4.933 -0.032

MgCO3 5.738e-006 5.744e-006 -5.241 -5.241 0.000

NaHCO3 1.396e-008 1.397e-008 -7.855 -7.855 0.000

NaCO3- 3.183e-009 2.955e-009 -8.497 -8.529 -0.032

Ca 1.104e-003

Ca+2 1.041e-003 7.787e-004 -2.982 -3.109 -0.126

CaHCO3+ 2.924e-005 2.719e-005 -4.534 -4.566 -0.032

CaCO3 2.142e-005 2.144e-005 -4.669 -4.669 0.000

CaSO4 1.143e-005 1.144e-005 -4.942 -4.942 0.000

CaOH+ 1.713e-008 1.590e-008 -7.766 -7.799 -0.032

CaHSO4+ 5.979e-013 5.549e-013 -12.223 -12.256 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 9.211e-028

H2 4.606e-028 4.611e-028 -27.337 -27.336 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.739e-009 1.614e-009 -8.760 -8.792 -0.032

KOH 1.313e-012 1.315e-012 -11.882 -11.881 0.000

Mg 5.184e-004

Mg+2 4.933e-004 3.701e-004 -3.307 -3.432 -0.125

MgHCO3+ 1.258e-005 1.168e-005 -4.900 -4.933 -0.032

MgSO4 6.535e-006 6.542e-006 -5.185 -5.184 0.000

MgCO3 5.738e-006 5.744e-006 -5.241 -5.241 0.000

MgOH+ 2.029e-007 1.883e-007 -6.693 -6.725 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.396e-008 1.397e-008 -7.855 -7.855 0.000

NaSO4- 3.672e-009 3.409e-009 -8.435 -8.467 -0.032

NaCO3- 3.183e-009 2.955e-009 -8.497 -8.529 -0.032

NaOH 7.530e-012 7.539e-012 -11.123 -11.123 0.000

O(0) 6.683e-004

O2 3.342e-004 3.345e-004 -3.476 -3.476 0.000

S(6) 1.154e-004

SO4-2 9.740e-005 7.266e-005 -4.011 -4.139 -0.127

CaSO4 1.143e-005 1.144e-005 -4.942 -4.942 0.000

MgSO4 6.535e-006 6.542e-006 -5.185 -5.184 0.000

NaSO4- 3.672e-009 3.409e-009 -8.435 -8.467 -0.032

KSO4- 1.739e-009 1.614e-009 -8.760 -8.792 -0.032

HSO4- 6.386e-011 5.928e-011 -10.195 -10.227 -0.032

CaHSO4+ 5.979e-013 5.549e-013 -12.223 -12.256 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.44 -7.91 -8.35 CaCO3

Calcite 0.58 -7.91 -8.49 CaCO3

CO2(g) -2.83 -4.32 -1.48 CO2

Dolomite 0.99 -16.14 -17.12 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.18 -27.34 -3.16 H2

H2O(g) -1.47 -0.00 1.47 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.57 -3.48 -2.90 O2

Initial solution 48. 29/8/2012 23:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.031e-003 3.031e-003

Ca 1.107e-003 1.107e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.183e-004 6.183e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.050

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 311

Density (g/cm3) = 0.99690

Activity of water = 1.000

Ionic strength = 4.821e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.038e-003

Total CO2 (mol/kg) = 3.038e-003

Temperature (deg C) = 26.360

Electrical balance (eq) = -5.455e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.86

Iterations = 7

Total H = 1.110154e+002

Total O = 5.551636e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.4805 0.7417

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.342e-006 1.244e-006 -5.872 -5.905 -0.033

H+ 9.537e-009 8.913e-009 -8.021 -8.050 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.038e-003

HCO3- 2.899e-003 2.696e-003 -2.538 -2.569 -0.032

CO2 5.309e-005 5.315e-005 -4.275 -4.274 0.000

CaHCO3+ 2.952e-005 2.745e-005 -4.530 -4.561 -0.032

CaCO3 1.967e-005 1.969e-005 -4.706 -4.706 0.000

CO3-2 1.949e-005 1.457e-005 -4.710 -4.836 -0.126

MgHCO3+ 1.266e-005 1.175e-005 -4.897 -4.930 -0.032

MgCO3 5.251e-006 5.257e-006 -5.280 -5.279 0.000

NaHCO3 1.404e-008 1.406e-008 -7.853 -7.852 0.000

NaCO3- 2.903e-009 2.694e-009 -8.537 -8.570 -0.032

Ca 1.107e-003

Ca+2 1.047e-003 7.822e-004 -2.980 -3.107 -0.126

CaHCO3+ 2.952e-005 2.745e-005 -4.530 -4.561 -0.032

CaCO3 1.967e-005 1.969e-005 -4.706 -4.706 0.000

CaSO4 1.146e-005 1.148e-005 -4.941 -4.940 0.000

CaOH+ 1.569e-008 1.456e-008 -7.804 -7.837 -0.032

CaHSO4+ 6.569e-013 6.097e-013 -12.183 -12.215 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.311e-005 -4.242 -4.275 -0.033

H(0) 1.108e-027

H2 5.542e-028 5.548e-028 -27.256 -27.256 0.000

K 3.326e-006

K+ 3.324e-006 3.082e-006 -5.478 -5.511 -0.033

KSO4- 1.735e-009 1.610e-009 -8.761 -8.793 -0.032

KOH 1.198e-012 1.199e-012 -11.922 -11.921 0.000

Mg 5.184e-004

Mg+2 4.938e-004 3.703e-004 -3.306 -3.431 -0.125

MgHCO3+ 1.266e-005 1.175e-005 -4.897 -4.930 -0.032

MgSO4 6.519e-006 6.526e-006 -5.186 -5.185 0.000

MgCO3 5.251e-006 5.257e-006 -5.280 -5.279 0.000

MgOH+ 1.836e-007 1.704e-007 -6.736 -6.768 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.404e-008 1.406e-008 -7.853 -7.852 0.000

NaSO4- 3.668e-009 3.404e-009 -8.436 -8.468 -0.032

NaCO3- 2.903e-009 2.694e-009 -8.537 -8.570 -0.032

NaOH 6.867e-012 6.875e-012 -11.163 -11.163 0.000

O(0) 6.183e-004

O2 3.091e-004 3.095e-004 -3.510 -3.509 0.000

S(6) 1.154e-004

SO4-2 9.738e-005 7.261e-005 -4.012 -4.139 -0.127

CaSO4 1.146e-005 1.148e-005 -4.941 -4.940 0.000

MgSO4 6.519e-006 6.526e-006 -5.186 -5.185 0.000

NaSO4- 3.668e-009 3.404e-009 -8.436 -8.468 -0.032

KSO4- 1.735e-009 1.610e-009 -8.761 -8.793 -0.032

HSO4- 6.985e-011 6.483e-011 -10.156 -10.188 -0.032

CaHSO4+ 6.569e-013 6.097e-013 -12.183 -12.215 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.40 -7.94 -8.34 CaCO3

Calcite 0.54 -7.94 -8.49 CaCO3

CO2(g) -2.79 -4.27 -1.48 CO2

Dolomite 0.91 -16.21 -17.12 CaMg(CO3)2

Gypsum -2.66 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.10 -27.26 -3.16 H2

H2O(g) -1.48 -0.00 1.47 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.61 -3.51 -2.90 O2

Initial solution 49. 29/8/2012 23:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.052e-003 3.052e-003

Ca 1.115e-003 1.115e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.920e-004 5.920e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.990

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 313

Density (g/cm3) = 0.99693

Activity of water = 1.000

Ionic strength = 4.852e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.073e-003

Total CO2 (mol/kg) = 3.073e-003

Temperature (deg C) = 26.270

Electrical balance (eq) = -6.040e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.95

Iterations = 7

Total H = 1.110154e+002

Total O = 5.551643e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.5432 0.7452

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.161e-006 1.076e-006 -5.935 -5.968 -0.033

H+ 1.095e-008 1.023e-008 -7.961 -7.990 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.073e-003

HCO3- 2.930e-003 2.724e-003 -2.533 -2.565 -0.032

CO2 6.166e-005 6.173e-005 -4.210 -4.210 0.000

CaHCO3+ 3.003e-005 2.792e-005 -4.522 -4.554 -0.032

CaCO3 1.739e-005 1.740e-005 -4.760 -4.759 0.000

CO3-2 1.713e-005 1.280e-005 -4.766 -4.893 -0.127

MgHCO3+ 1.280e-005 1.187e-005 -4.893 -4.925 -0.032

MgCO3 4.609e-006 4.614e-006 -5.336 -5.336 0.000

NaHCO3 1.419e-008 1.420e-008 -7.848 -7.848 0.000

NaCO3- 2.539e-009 2.356e-009 -8.595 -8.628 -0.032

Ca 1.115e-003

Ca+2 1.056e-003 7.885e-004 -2.976 -3.103 -0.127

CaHCO3+ 3.003e-005 2.792e-005 -4.522 -4.554 -0.032

CaCO3 1.739e-005 1.740e-005 -4.760 -4.759 0.000

CaSO4 1.153e-005 1.154e-005 -4.938 -4.938 0.000

CaOH+ 1.378e-008 1.279e-008 -7.861 -7.893 -0.032

CaHSO4+ 7.579e-013 7.033e-013 -12.120 -12.153 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.310e-005 -4.242 -4.275 -0.033

H(0) 1.462e-027

H2 7.312e-028 7.320e-028 -27.136 -27.135 0.000

K 3.326e-006

K+ 3.324e-006 3.082e-006 -5.478 -5.511 -0.033

KSO4- 1.730e-009 1.605e-009 -8.762 -8.794 -0.032

KOH 1.043e-012 1.044e-012 -11.982 -11.981 0.000

Mg 5.184e-004

Mg+2 4.943e-004 3.704e-004 -3.306 -3.431 -0.125

MgHCO3+ 1.280e-005 1.187e-005 -4.893 -4.925 -0.032

MgSO4 6.498e-006 6.506e-006 -5.187 -5.187 0.000

MgCO3 4.609e-006 4.614e-006 -5.336 -5.336 0.000

MgOH+ 1.588e-007 1.473e-007 -6.799 -6.832 -0.032

Na 1.001e-005

Na+ 9.987e-006 9.273e-006 -5.001 -5.033 -0.032

NaHCO3 1.419e-008 1.420e-008 -7.848 -7.848 0.000

NaSO4- 3.661e-009 3.398e-009 -8.436 -8.469 -0.032

NaCO3- 2.539e-009 2.356e-009 -8.595 -8.628 -0.032

NaOH 5.980e-012 5.987e-012 -11.223 -11.223 0.000

O(0) 5.920e-004

O2 2.960e-004 2.963e-004 -3.529 -3.528 0.000

S(6) 1.154e-004

SO4-2 9.733e-005 7.252e-005 -4.012 -4.140 -0.128

CaSO4 1.153e-005 1.154e-005 -4.938 -4.938 0.000

MgSO4 6.498e-006 6.506e-006 -5.187 -5.187 0.000

NaSO4- 3.661e-009 3.398e-009 -8.436 -8.469 -0.032

KSO4- 1.730e-009 1.605e-009 -8.762 -8.794 -0.032

HSO4- 7.995e-011 7.419e-011 -10.097 -10.130 -0.032

CaHSO4+ 7.579e-013 7.033e-013 -12.120 -12.153 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.24 -4.37 CaSO4

Aragonite 0.35 -8.00 -8.34 CaCO3

Calcite 0.49 -8.00 -8.49 CaCO3

CO2(g) -2.73 -4.21 -1.48 CO2

Dolomite 0.80 -16.32 -17.12 CaMg(CO3)2

Gypsum -2.66 -7.24 -4.58 CaSO4:2H2O

H2(g) -23.98 -27.14 -3.16 H2

H2O(g) -1.48 -0.00 1.48 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -0.63 -3.53 -2.90 O2

Initial solution 50. 30/8/2012 00:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.062e-003 3.062e-003

Ca 1.119e-003 1.119e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.645e-004 5.645e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.940

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 314

Density (g/cm3) = 0.99692

Activity of water = 1.000

Ionic strength = 4.868e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.096e-003

Total CO2 (mol/kg) = 3.096e-003

Temperature (deg C) = 26.310

Electrical balance (eq) = -6.324e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.99

Iterations = 7

Total H = 1.110154e+002

Total O = 5.551646e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.5848 0.7477

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.038e-006 9.620e-007 -5.984 -6.017 -0.033

H+ 1.229e-008 1.148e-008 -7.910 -7.940 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.096e-003

HCO3- 2.948e-003 2.740e-003 -2.531 -2.562 -0.032

CO2 6.957e-005 6.964e-005 -4.158 -4.157 0.000

CaHCO3+ 3.037e-005 2.823e-005 -4.518 -4.549 -0.032

CaCO3 1.568e-005 1.570e-005 -4.805 -4.804 0.000

CO3-2 1.538e-005 1.149e-005 -4.813 -4.940 -0.127

MgHCO3+ 1.288e-005 1.195e-005 -4.890 -4.923 -0.033

MgCO3 4.140e-006 4.144e-006 -5.383 -5.383 0.000

NaHCO3 1.427e-008 1.429e-008 -7.846 -7.845 0.000

NaCO3- 2.283e-009 2.118e-009 -8.642 -8.674 -0.033

Ca 1.119e-003

Ca+2 1.061e-003 7.919e-004 -2.974 -3.101 -0.127

CaHCO3+ 3.037e-005 2.823e-005 -4.518 -4.549 -0.032

CaCO3 1.568e-005 1.570e-005 -4.805 -4.804 0.000

CaSO4 1.158e-005 1.159e-005 -4.936 -4.936 0.000

CaOH+ 1.234e-008 1.145e-008 -7.909 -7.941 -0.033

CaHSO4+ 8.542e-013 7.925e-013 -12.068 -12.101 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.310e-005 -4.242 -4.275 -0.033

H(0) 1.840e-027

H2 9.202e-028 9.212e-028 -27.036 -27.036 0.000

K 3.326e-006

K+ 3.324e-006 3.081e-006 -5.478 -5.511 -0.033

KSO4- 1.730e-009 1.605e-009 -8.762 -8.795 -0.033

KOH 9.294e-013 9.305e-013 -12.032 -12.031 0.000

Mg 5.184e-004

Mg+2 4.947e-004 3.705e-004 -3.306 -3.431 -0.126

MgHCO3+ 1.288e-005 1.195e-005 -4.890 -4.923 -0.033

MgSO4 6.501e-006 6.509e-006 -5.187 -5.187 0.000

MgCO3 4.140e-006 4.144e-006 -5.383 -5.383 0.000

MgOH+ 1.421e-007 1.318e-007 -6.848 -6.880 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.272e-006 -5.001 -5.033 -0.032

NaHCO3 1.427e-008 1.429e-008 -7.846 -7.845 0.000

NaSO4- 3.659e-009 3.395e-009 -8.437 -8.469 -0.033

NaCO3- 2.283e-009 2.118e-009 -8.642 -8.674 -0.033

NaOH 5.329e-012 5.335e-012 -11.273 -11.273 0.000

O(0) 5.645e-004

O2 2.823e-004 2.826e-004 -3.549 -3.549 0.000

S(6) 1.154e-004

SO4-2 9.729e-005 7.245e-005 -4.012 -4.140 -0.128

CaSO4 1.158e-005 1.159e-005 -4.936 -4.936 0.000

MgSO4 6.501e-006 6.509e-006 -5.187 -5.187 0.000

NaSO4- 3.659e-009 3.395e-009 -8.437 -8.469 -0.033

KSO4- 1.730e-009 1.605e-009 -8.762 -8.795 -0.033

HSO4- 8.971e-011 8.324e-011 -10.047 -10.080 -0.033

CaHSO4+ 8.542e-013 7.925e-013 -12.068 -12.101 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.87 -7.24 -4.37 CaSO4

Aragonite 0.30 -8.04 -8.34 CaCO3

Calcite 0.45 -8.04 -8.49 CaCO3

CO2(g) -2.67 -4.16 -1.48 CO2

Dolomite 0.71 -16.41 -17.12 CaMg(CO3)2

Gypsum -2.66 -7.24 -4.58 CaSO4:2H2O

H2(g) -23.88 -27.04 -3.16 H2

H2O(g) -1.48 -0.00 1.48 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -0.65 -3.55 -2.90 O2

Initial solution 51. 30/8/2012 00:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.062e-003 3.062e-003

Ca 1.119e-003 1.119e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.389e-004 5.389e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.890

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 313

Density (g/cm3) = 0.99695

Activity of water = 1.000

Ionic strength = 4.873e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.108e-003

Total CO2 (mol/kg) = 3.108e-003

Temperature (deg C) = 26.180

Electrical balance (eq) = -6.324e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.99

Iterations = 7

Total H = 1.110154e+002

Total O = 5.551647e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.6404 0.7507

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.161e-007 8.491e-007 -6.038 -6.071 -0.033

H+ 1.379e-008 1.288e-008 -7.860 -7.890 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.108e-003

HCO3- 2.955e-003 2.747e-003 -2.529 -2.561 -0.032

CO2 7.838e-005 7.846e-005 -4.106 -4.105 0.000

CaHCO3+ 3.043e-005 2.829e-005 -4.517 -4.548 -0.032

CaCO3 1.396e-005 1.397e-005 -4.855 -4.855 0.000

CO3-2 1.371e-005 1.024e-005 -4.863 -4.990 -0.127

MgHCO3+ 1.292e-005 1.199e-005 -4.889 -4.921 -0.033

MgCO3 3.685e-006 3.690e-006 -5.434 -5.433 0.000

NaHCO3 1.431e-008 1.432e-008 -7.844 -7.844 0.000

NaCO3- 2.022e-009 1.876e-009 -8.694 -8.727 -0.033

Ca 1.119e-003

Ca+2 1.063e-003 7.931e-004 -2.974 -3.101 -0.127

CaHCO3+ 3.043e-005 2.829e-005 -4.517 -4.548 -0.032

CaCO3 1.396e-005 1.397e-005 -4.855 -4.855 0.000

CaSO4 1.158e-005 1.159e-005 -4.936 -4.936 0.000

CaOH+ 1.101e-008 1.022e-008 -7.958 -7.991 -0.033

CaHSO4+ 9.571e-013 8.880e-013 -12.019 -12.052 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.310e-005 -4.242 -4.275 -0.033

H(0) 2.320e-027

H2 1.160e-027 1.161e-027 -26.936 -26.935 0.000

K 3.326e-006

K+ 3.324e-006 3.081e-006 -5.478 -5.511 -0.033

KSO4- 1.726e-009 1.601e-009 -8.763 -8.796 -0.033

KOH 8.283e-013 8.293e-013 -12.082 -12.081 0.000

Mg 5.184e-004

Mg+2 4.952e-004 3.709e-004 -3.305 -3.431 -0.126

MgHCO3+ 1.292e-005 1.199e-005 -4.889 -4.921 -0.033

MgSO4 6.486e-006 6.493e-006 -5.188 -5.188 0.000

MgCO3 3.685e-006 3.690e-006 -5.434 -5.433 0.000

MgOH+ 1.253e-007 1.162e-007 -6.902 -6.935 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.272e-006 -5.001 -5.033 -0.032

NaHCO3 1.431e-008 1.432e-008 -7.844 -7.844 0.000

NaSO4- 3.656e-009 3.392e-009 -8.437 -8.470 -0.033

NaCO3- 2.022e-009 1.876e-009 -8.694 -8.727 -0.033

NaOH 4.750e-012 4.755e-012 -11.323 -11.323 0.000

O(0) 5.389e-004

O2 2.694e-004 2.697e-004 -3.570 -3.569 0.000

S(6) 1.154e-004

SO4-2 9.730e-005 7.246e-005 -4.012 -4.140 -0.128

CaSO4 1.158e-005 1.159e-005 -4.936 -4.936 0.000

MgSO4 6.486e-006 6.493e-006 -5.188 -5.188 0.000

NaSO4- 3.656e-009 3.392e-009 -8.437 -8.470 -0.033

KSO4- 1.726e-009 1.601e-009 -8.763 -8.796 -0.033

HSO4- 1.004e-010 9.313e-011 -9.998 -10.031 -0.033

CaHSO4+ 9.571e-013 8.880e-013 -12.019 -12.052 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.87 -7.24 -4.37 CaSO4

Aragonite 0.25 -8.09 -8.34 CaCO3

Calcite 0.40 -8.09 -8.49 CaCO3

CO2(g) -2.62 -4.11 -1.48 CO2

Dolomite 0.61 -16.51 -17.12 CaMg(CO3)2

Gypsum -2.66 -7.24 -4.58 CaSO4:2H2O

H2(g) -23.78 -26.94 -3.16 H2

H2O(g) -1.48 -0.00 1.48 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -0.67 -3.57 -2.90 O2

Initial solution 52. 30/8/2012 00:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.083e-003 3.083e-003

Ca 1.126e-003 1.126e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.151e-004 5.151e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.850

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 315

Density (g/cm3) = 0.99695

Activity of water = 1.000

Ionic strength = 4.900e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.140e-003

Total CO2 (mol/kg) = 3.140e-003

Temperature (deg C) = 26.180

Electrical balance (eq) = -6.892e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.07

Iterations = 7

Total H = 1.110155e+002

Total O = 5.551653e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.6755 0.7528

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.356e-007 7.744e-007 -6.078 -6.111 -0.033

H+ 1.512e-008 1.413e-008 -7.820 -7.850 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.140e-003

HCO3- 2.980e-003 2.770e-003 -2.526 -2.558 -0.032

CO2 8.665e-005 8.675e-005 -4.062 -4.062 0.000

CaHCO3+ 3.090e-005 2.872e-005 -4.510 -4.542 -0.032

MgHCO3+ 1.303e-005 1.208e-005 -4.885 -4.918 -0.033

CaCO3 1.292e-005 1.294e-005 -4.889 -4.888 0.000

CO3-2 1.262e-005 9.415e-006 -4.899 -5.026 -0.127

MgCO3 3.388e-006 3.392e-006 -5.470 -5.470 0.000

NaHCO3 1.442e-008 1.444e-008 -7.841 -7.840 0.000

NaCO3- 1.859e-009 1.724e-009 -8.731 -8.763 -0.033

Ca 1.126e-003

Ca+2 1.071e-003 7.985e-004 -2.970 -3.098 -0.127

CaHCO3+ 3.090e-005 2.872e-005 -4.510 -4.542 -0.032

CaCO3 1.292e-005 1.294e-005 -4.889 -4.888 0.000

CaSO4 1.164e-005 1.166e-005 -4.934 -4.933 0.000

CaOH+ 1.011e-008 9.381e-009 -7.995 -8.028 -0.033

CaHSO4+ 1.055e-012 9.791e-013 -11.977 -12.009 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.308e-005 -4.242 -4.275 -0.033

H(0) 2.789e-027

H2 1.395e-027 1.396e-027 -26.856 -26.855 0.000

K 3.326e-006

K+ 3.324e-006 3.081e-006 -5.478 -5.511 -0.033

KSO4- 1.724e-009 1.599e-009 -8.764 -8.796 -0.033

KOH 7.553e-013 7.562e-013 -12.122 -12.121 0.000

Mg 5.184e-004

Mg+2 4.954e-004 3.708e-004 -3.305 -3.431 -0.126

MgHCO3+ 1.303e-005 1.208e-005 -4.885 -4.918 -0.033

MgSO4 6.475e-006 6.483e-006 -5.189 -5.188 0.000

MgCO3 3.388e-006 3.392e-006 -5.470 -5.470 0.000

MgOH+ 1.142e-007 1.060e-007 -6.942 -6.975 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.270e-006 -5.001 -5.033 -0.032

NaHCO3 1.442e-008 1.444e-008 -7.841 -7.840 0.000

NaSO4- 3.652e-009 3.387e-009 -8.438 -8.470 -0.033

NaCO3- 1.859e-009 1.724e-009 -8.731 -8.763 -0.033

NaOH 4.331e-012 4.336e-012 -11.363 -11.363 0.000

O(0) 5.151e-004

O2 2.576e-004 2.579e-004 -3.589 -3.589 0.000

S(6) 1.154e-004

SO4-2 9.725e-005 7.236e-005 -4.012 -4.140 -0.128

CaSO4 1.164e-005 1.166e-005 -4.934 -4.933 0.000

MgSO4 6.475e-006 6.483e-006 -5.189 -5.188 0.000

NaSO4- 3.652e-009 3.387e-009 -8.438 -8.470 -0.033

KSO4- 1.724e-009 1.599e-009 -8.764 -8.796 -0.033

HSO4- 1.099e-010 1.020e-010 -9.959 -9.991 -0.033

CaHSO4+ 1.055e-012 9.791e-013 -11.977 -12.009 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.87 -7.24 -4.37 CaSO4

Aragonite 0.22 -8.12 -8.34 CaCO3

Calcite 0.36 -8.12 -8.49 CaCO3

CO2(g) -2.58 -4.06 -1.48 CO2

Dolomite 0.54 -16.58 -17.12 CaMg(CO3)2

Gypsum -2.66 -7.24 -4.58 CaSO4:2H2O

H2(g) -23.70 -26.86 -3.16 H2

H2O(g) -1.48 -0.00 1.48 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -0.69 -3.59 -2.90 O2

Initial solution 53. 30/8/2012 00:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.104e-003 3.104e-003

Ca 1.134e-003 1.134e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.926e-004 4.926e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.820

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 315

Density (g/cm3) = 0.99701

Activity of water = 1.000

Ionic strength = 4.926e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.169e-003

Total CO2 (mol/kg) = 3.169e-003

Temperature (deg C) = 25.960

Electrical balance (eq) = -7.444e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.15

Iterations = 7

Total H = 1.110155e+002

Total O = 5.551659e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.7187 0.7548

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 7.673e-007 7.109e-007 -6.115 -6.148 -0.033

H+ 1.621e-008 1.514e-008 -7.790 -7.820 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.169e-003

HCO3- 3.004e-003 2.792e-003 -2.522 -2.554 -0.032

CO2 9.381e-005 9.392e-005 -4.028 -4.027 0.000

CaHCO3+ 3.126e-005 2.905e-005 -4.505 -4.537 -0.032

MgHCO3+ 1.311e-005 1.216e-005 -4.882 -4.915 -0.033

CaCO3 1.213e-005 1.214e-005 -4.916 -4.916 0.000

CO3-2 1.182e-005 8.817e-006 -4.927 -5.055 -0.127

MgCO3 3.162e-006 3.165e-006 -5.500 -5.500 0.000

NaHCO3 1.454e-008 1.455e-008 -7.838 -7.837 0.000

NaCO3- 1.722e-009 1.597e-009 -8.764 -8.797 -0.033

Ca 1.134e-003

Ca+2 1.078e-003 8.039e-004 -2.967 -3.095 -0.128

CaHCO3+ 3.126e-005 2.905e-005 -4.505 -4.537 -0.032

CaCO3 1.213e-005 1.214e-005 -4.916 -4.916 0.000

CaSO4 1.169e-005 1.170e-005 -4.932 -4.932 0.000

CaOH+ 9.503e-009 8.814e-009 -8.022 -8.055 -0.033

CaHSO4+ 1.133e-012 1.050e-012 -11.946 -11.979 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.308e-005 -4.242 -4.275 -0.033

H(0) 3.209e-027

H2 1.605e-027 1.606e-027 -26.795 -26.794 0.000

K 3.326e-006

K+ 3.324e-006 3.080e-006 -5.478 -5.511 -0.033

KSO4- 1.716e-009 1.591e-009 -8.765 -8.798 -0.033

KOH 7.048e-013 7.056e-013 -12.152 -12.151 0.000

Mg 5.184e-004

Mg+2 4.956e-004 3.707e-004 -3.305 -3.431 -0.126

MgHCO3+ 1.311e-005 1.216e-005 -4.882 -4.915 -0.033

MgSO4 6.434e-006 6.441e-006 -5.192 -5.191 0.000

MgCO3 3.162e-006 3.165e-006 -5.500 -5.500 0.000

MgOH+ 1.045e-007 9.694e-008 -6.981 -7.014 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.269e-006 -5.001 -5.033 -0.032

NaHCO3 1.454e-008 1.455e-008 -7.838 -7.837 0.000

NaSO4- 3.644e-009 3.380e-009 -8.438 -8.471 -0.033

NaCO3- 1.722e-009 1.597e-009 -8.764 -8.797 -0.033

NaOH 4.041e-012 4.046e-012 -11.393 -11.393 0.000

O(0) 4.926e-004

O2 2.463e-004 2.466e-004 -3.609 -3.608 0.000

S(6) 1.154e-004

SO4-2 9.724e-005 7.232e-005 -4.012 -4.141 -0.129

CaSO4 1.169e-005 1.170e-005 -4.932 -4.932 0.000

MgSO4 6.434e-006 6.441e-006 -5.192 -5.191 0.000

NaSO4- 3.644e-009 3.380e-009 -8.438 -8.471 -0.033

KSO4- 1.716e-009 1.591e-009 -8.765 -8.798 -0.033

HSO4- 1.172e-010 1.087e-010 -9.931 -9.964 -0.033

CaHSO4+ 1.133e-012 1.050e-012 -11.946 -11.979 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.87 -7.24 -4.36 CaSO4

Aragonite 0.19 -8.15 -8.34 CaCO3

Calcite 0.34 -8.15 -8.49 CaCO3

CO2(g) -2.55 -4.03 -1.48 CO2

Dolomite 0.48 -16.64 -17.11 CaMg(CO3)2

Gypsum -2.65 -7.24 -4.58 CaSO4:2H2O

H2(g) -23.64 -26.79 -3.15 H2

H2O(g) -1.49 -0.00 1.49 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -0.71 -3.61 -2.90 O2

Initial solution 54. 30/8/2012 01:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.104e-003 3.104e-003

Ca 1.134e-003 1.134e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.670e-004 4.670e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.770

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 315

Density (g/cm3) = 0.99702

Activity of water = 1.000

Ionic strength = 4.930e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.184e-003

Total CO2 (mol/kg) = 3.184e-003

Temperature (deg C) = 25.920

Electrical balance (eq) = -7.444e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.15

Iterations = 7

Total H = 1.110155e+002

Total O = 5.551659e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.7662 0.7575

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 6.818e-007 6.317e-007 -6.166 -6.199 -0.033

H+ 1.818e-008 1.698e-008 -7.740 -7.770 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.184e-003

HCO3- 3.010e-003 2.797e-003 -2.521 -2.553 -0.032

CO2 1.055e-004 1.056e-004 -3.977 -3.976 0.000

CaHCO3+ 3.133e-005 2.912e-005 -4.504 -4.536 -0.032

MgHCO3+ 1.314e-005 1.219e-005 -4.881 -4.914 -0.033

CaCO3 1.082e-005 1.084e-005 -4.966 -4.965 0.000

CO3-2 1.055e-005 7.867e-006 -4.977 -5.104 -0.127

MgCO3 2.821e-006 2.824e-006 -5.550 -5.549 0.000

NaHCO3 1.456e-008 1.458e-008 -7.837 -7.836 0.000

NaCO3- 1.533e-009 1.422e-009 -8.814 -8.847 -0.033

Ca 1.134e-003

Ca+2 1.080e-003 8.047e-004 -2.967 -3.094 -0.128

CaHCO3+ 3.133e-005 2.912e-005 -4.504 -4.536 -0.032

CaSO4 1.170e-005 1.171e-005 -4.932 -4.931 0.000

CaCO3 1.082e-005 1.084e-005 -4.966 -4.965 0.000

CaOH+ 8.479e-009 7.864e-009 -8.072 -8.104 -0.033

CaHSO4+ 1.271e-012 1.179e-012 -11.896 -11.929 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.308e-005 -4.242 -4.275 -0.033

H(0) 4.042e-027

H2 2.021e-027 2.023e-027 -26.694 -26.694 0.000

K 3.326e-006

K+ 3.324e-006 3.080e-006 -5.478 -5.511 -0.033

KSO4- 1.715e-009 1.590e-009 -8.766 -8.799 -0.033

KOH 6.281e-013 6.288e-013 -12.202 -12.201 0.000

Mg 5.184e-004

Mg+2 4.959e-004 3.709e-004 -3.305 -3.431 -0.126

MgHCO3+ 1.314e-005 1.219e-005 -4.881 -4.914 -0.033

MgSO4 6.430e-006 6.437e-006 -5.192 -5.191 0.000

MgCO3 2.821e-006 2.824e-006 -5.550 -5.549 0.000

MgOH+ 9.287e-008 8.614e-008 -7.032 -7.065 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.269e-006 -5.001 -5.033 -0.032

NaHCO3 1.456e-008 1.458e-008 -7.837 -7.836 0.000

NaSO4- 3.643e-009 3.379e-009 -8.439 -8.471 -0.033

NaCO3- 1.533e-009 1.422e-009 -8.814 -8.847 -0.033

NaOH 3.602e-012 3.606e-012 -11.444 -11.443 0.000

O(0) 4.670e-004

O2 2.335e-004 2.338e-004 -3.632 -3.631 0.000

S(6) 1.154e-004

SO4-2 9.724e-005 7.231e-005 -4.012 -4.141 -0.129

CaSO4 1.170e-005 1.171e-005 -4.932 -4.931 0.000

MgSO4 6.430e-006 6.437e-006 -5.192 -5.191 0.000

NaSO4- 3.643e-009 3.379e-009 -8.439 -8.471 -0.033

KSO4- 1.715e-009 1.590e-009 -8.766 -8.799 -0.033

HSO4- 1.313e-010 1.218e-010 -9.882 -9.914 -0.033

CaHSO4+ 1.271e-012 1.179e-012 -11.896 -11.929 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.87 -7.24 -4.36 CaSO4

Aragonite 0.14 -8.20 -8.34 CaCO3

Calcite 0.29 -8.20 -8.49 CaCO3

CO2(g) -2.50 -3.98 -1.48 CO2

Dolomite 0.38 -16.73 -17.11 CaMg(CO3)2

Gypsum -2.65 -7.24 -4.58 CaSO4:2H2O

H2(g) -23.54 -26.69 -3.15 H2

H2O(g) -1.49 -0.00 1.49 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -0.73 -3.63 -2.90 O2

Initial solution 55. 30/8/2012 01:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.124e-003 3.124e-003

Ca 1.141e-003 1.141e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.395e-004 4.395e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.760

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 316

Density (g/cm3) = 0.99705

Activity of water = 1.000

Ionic strength = 4.955e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.209e-003

Total CO2 (mol/kg) = 3.209e-003

Temperature (deg C) = 25.820

Electrical balance (eq) = -8.028e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.23

Iterations = 7

Total H = 1.110155e+002

Total O = 5.551664e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.7779 0.7580

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 6.614e-007 6.127e-007 -6.180 -6.213 -0.033

H+ 1.861e-008 1.738e-008 -7.730 -7.760 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.209e-003

HCO3- 3.031e-003 2.816e-003 -2.518 -2.550 -0.032

CO2 1.088e-004 1.090e-004 -3.963 -3.963 0.000

CaHCO3+ 3.170e-005 2.945e-005 -4.499 -4.531 -0.032

MgHCO3+ 1.322e-005 1.226e-005 -4.879 -4.911 -0.033

CaCO3 1.067e-005 1.068e-005 -4.972 -4.971 0.000

CO3-2 1.037e-005 7.726e-006 -4.984 -5.112 -0.128

MgCO3 2.764e-006 2.767e-006 -5.558 -5.558 0.000

NaHCO3 1.466e-008 1.468e-008 -7.834 -7.833 0.000

NaCO3- 1.498e-009 1.389e-009 -8.824 -8.857 -0.033

Ca 1.141e-003

Ca+2 1.087e-003 8.096e-004 -2.964 -3.092 -0.128

CaHCO3+ 3.170e-005 2.945e-005 -4.499 -4.531 -0.032

CaSO4 1.175e-005 1.176e-005 -4.930 -4.930 0.000

CaCO3 1.067e-005 1.068e-005 -4.972 -4.971 0.000

CaOH+ 8.337e-009 7.731e-009 -8.079 -8.112 -0.033

CaHSO4+ 1.305e-012 1.210e-012 -11.885 -11.917 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.307e-005 -4.242 -4.275 -0.033

H(0) 4.236e-027

H2 2.118e-027 2.121e-027 -26.674 -26.674 0.000

K 3.326e-006

K+ 3.324e-006 3.080e-006 -5.478 -5.511 -0.033

KSO4- 1.710e-009 1.586e-009 -8.767 -8.800 -0.033

KOH 6.137e-013 6.144e-013 -12.212 -12.212 0.000

Mg 5.184e-004

Mg+2 4.959e-004 3.707e-004 -3.305 -3.431 -0.126

MgHCO3+ 1.322e-005 1.226e-005 -4.879 -4.911 -0.033

MgSO4 6.404e-006 6.412e-006 -5.194 -5.193 0.000

MgCO3 2.764e-006 2.767e-006 -5.558 -5.558 0.000

MgOH+ 8.991e-008 8.338e-008 -7.046 -7.079 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.267e-006 -5.001 -5.033 -0.032

NaHCO3 1.466e-008 1.468e-008 -7.834 -7.833 0.000

NaSO4- 3.638e-009 3.373e-009 -8.439 -8.472 -0.033

NaCO3- 1.498e-009 1.389e-009 -8.824 -8.857 -0.033

NaOH 3.519e-012 3.523e-012 -11.454 -11.453 0.000

O(0) 4.395e-004

O2 2.197e-004 2.200e-004 -3.658 -3.658 0.000

S(6) 1.154e-004

SO4-2 9.721e-005 7.225e-005 -4.012 -4.141 -0.129

CaSO4 1.175e-005 1.176e-005 -4.930 -4.930 0.000

MgSO4 6.404e-006 6.412e-006 -5.194 -5.193 0.000

NaSO4- 3.638e-009 3.373e-009 -8.439 -8.472 -0.033

KSO4- 1.710e-009 1.586e-009 -8.767 -8.800 -0.033

HSO4- 1.340e-010 1.243e-010 -9.873 -9.906 -0.033

CaHSO4+ 1.305e-012 1.210e-012 -11.885 -11.917 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.87 -7.23 -4.36 CaSO4

Aragonite 0.14 -8.20 -8.34 CaCO3

Calcite 0.28 -8.20 -8.48 CaCO3

CO2(g) -2.49 -3.96 -1.48 CO2

Dolomite 0.36 -16.75 -17.11 CaMg(CO3)2

Gypsum -2.65 -7.23 -4.58 CaSO4:2H2O

H2(g) -23.52 -26.67 -3.15 H2

H2O(g) -1.49 -0.00 1.49 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -0.76 -3.66 -2.90 O2

Initial solution 56. 30/8/2012 01:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.135e-003 3.135e-003

Ca 1.145e-003 1.145e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.451e-004 3.451e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.710

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 317

Density (g/cm3) = 0.99707

Activity of water = 1.000

Ionic strength = 4.970e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.235e-003

Total CO2 (mol/kg) = 3.235e-003

Temperature (deg C) = 25.760

Electrical balance (eq) = -8.296e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.27

Iterations = 7

Total H = 1.110155e+002

Total O = 5.551661e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8066 0.7595

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 5.869e-007 5.436e-007 -6.231 -6.265 -0.033

H+ 2.088e-008 1.950e-008 -7.680 -7.710 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.235e-003

HCO3- 3.046e-003 2.830e-003 -2.516 -2.548 -0.032

CO2 1.228e-004 1.229e-004 -3.911 -3.910 0.000

CaHCO3+ 3.195e-005 2.968e-005 -4.496 -4.528 -0.032

MgHCO3+ 1.329e-005 1.232e-005 -4.877 -4.909 -0.033

CaCO3 9.571e-006 9.582e-006 -5.019 -5.019 0.000

CO3-2 9.276e-006 6.911e-006 -5.033 -5.160 -0.128

MgCO3 2.471e-006 2.474e-006 -5.607 -5.607 0.000

NaHCO3 1.473e-008 1.475e-008 -7.832 -7.831 0.000

NaCO3- 1.336e-009 1.239e-009 -8.874 -8.907 -0.033

Ca 1.145e-003

Ca+2 1.091e-003 8.127e-004 -2.962 -3.090 -0.128

CaHCO3+ 3.195e-005 2.968e-005 -4.496 -4.528 -0.032

CaSO4 1.178e-005 1.179e-005 -4.929 -4.928 0.000

CaCO3 9.571e-006 9.582e-006 -5.019 -5.019 0.000

CaOH+ 7.460e-009 6.917e-009 -8.127 -8.160 -0.033

CaHSO4+ 1.467e-012 1.360e-012 -11.834 -11.866 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.306e-005 -4.242 -4.275 -0.033

H(0) 5.336e-027

H2 2.668e-027 2.671e-027 -26.574 -26.573 0.000

K 3.326e-006

K+ 3.324e-006 3.079e-006 -5.478 -5.512 -0.033

KSO4- 1.707e-009 1.583e-009 -8.768 -8.800 -0.033

KOH 5.469e-013 5.475e-013 -12.262 -12.262 0.000

Mg 5.184e-004

Mg+2 4.962e-004 3.707e-004 -3.304 -3.431 -0.127

MgHCO3+ 1.329e-005 1.232e-005 -4.877 -4.909 -0.033

MgSO4 6.392e-006 6.399e-006 -5.194 -5.194 0.000

MgCO3 2.471e-006 2.474e-006 -5.607 -5.607 0.000

MgOH+ 7.972e-008 7.392e-008 -7.098 -7.131 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.267e-006 -5.001 -5.033 -0.033

NaHCO3 1.473e-008 1.475e-008 -7.832 -7.831 0.000

NaSO4- 3.634e-009 3.370e-009 -8.440 -8.472 -0.033

NaCO3- 1.336e-009 1.239e-009 -8.874 -8.907 -0.033

NaOH 3.136e-012 3.140e-012 -11.504 -11.503 0.000

O(0) 3.451e-004

O2 1.725e-004 1.727e-004 -3.763 -3.763 0.000

S(6) 1.154e-004

SO4-2 9.719e-005 7.220e-005 -4.012 -4.141 -0.129

CaSO4 1.178e-005 1.179e-005 -4.929 -4.928 0.000

MgSO4 6.392e-006 6.399e-006 -5.194 -5.194 0.000

NaSO4- 3.634e-009 3.370e-009 -8.440 -8.472 -0.033

KSO4- 1.707e-009 1.583e-009 -8.768 -8.800 -0.033

HSO4- 1.501e-010 1.392e-010 -9.824 -9.856 -0.033

CaHSO4+ 1.467e-012 1.360e-012 -11.834 -11.866 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.87 -7.23 -4.36 CaSO4

Aragonite 0.09 -8.25 -8.34 CaCO3

Calcite 0.23 -8.25 -8.48 CaCO3

CO2(g) -2.43 -3.91 -1.48 CO2

Dolomite 0.27 -16.84 -17.11 CaMg(CO3)2

Gypsum -2.65 -7.23 -4.58 CaSO4:2H2O

H2(g) -23.42 -26.57 -3.15 H2

H2O(g) -1.49 -0.00 1.49 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -0.86 -3.76 -2.90 O2

Initial solution 57. 30/8/2012 01:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.145e-003 3.145e-003

Ca 1.149e-003 1.149e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.132e-004 3.132e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.700

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 317

Density (g/cm3) = 0.99709

Activity of water = 1.000

Ionic strength = 4.982e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.250e-003

Total CO2 (mol/kg) = 3.250e-003

Temperature (deg C) = 25.670

Electrical balance (eq) = -8.596e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.31

Iterations = 7

Total H = 1.110155e+002

Total O = 5.551662e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8135 0.7597

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 5.697e-007 5.277e-007 -6.244 -6.278 -0.033

H+ 2.137e-008 1.995e-008 -7.670 -7.700 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.250e-003

HCO3- 3.057e-003 2.840e-003 -2.515 -2.547 -0.032

CO2 1.262e-004 1.264e-004 -3.899 -3.898 0.000

CaHCO3+ 3.212e-005 2.984e-005 -4.493 -4.525 -0.032

MgHCO3+ 1.333e-005 1.236e-005 -4.875 -4.908 -0.033

CaCO3 9.382e-006 9.393e-006 -5.028 -5.027 0.000

CO3-2 9.083e-006 6.766e-006 -5.042 -5.170 -0.128

MgCO3 2.415e-006 2.418e-006 -5.617 -5.617 0.000

NaHCO3 1.478e-008 1.480e-008 -7.830 -7.830 0.000

NaCO3- 1.302e-009 1.207e-009 -8.885 -8.918 -0.033

Ca 1.149e-003

Ca+2 1.095e-003 8.153e-004 -2.961 -3.089 -0.128

CaHCO3+ 3.212e-005 2.984e-005 -4.493 -4.525 -0.032

CaSO4 1.180e-005 1.181e-005 -4.928 -4.928 0.000

CaCO3 9.382e-006 9.393e-006 -5.028 -5.027 0.000

CaOH+ 7.313e-009 6.781e-009 -8.136 -8.169 -0.033

CaHSO4+ 1.502e-012 1.393e-012 -11.823 -11.856 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.306e-005 -4.242 -4.275 -0.033

H(0) 5.593e-027

H2 2.796e-027 2.800e-027 -26.553 -26.553 0.000

K 3.326e-006

K+ 3.324e-006 3.079e-006 -5.478 -5.512 -0.033

KSO4- 1.704e-009 1.580e-009 -8.769 -8.801 -0.033

KOH 5.344e-013 5.350e-013 -12.272 -12.272 0.000

Mg 5.184e-004

Mg+2 4.962e-004 3.707e-004 -3.304 -3.431 -0.127

MgHCO3+ 1.333e-005 1.236e-005 -4.875 -4.908 -0.033

MgSO4 6.373e-006 6.381e-006 -5.196 -5.195 0.000

MgCO3 2.415e-006 2.418e-006 -5.617 -5.617 0.000

MgOH+ 7.727e-008 7.164e-008 -7.112 -7.145 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.266e-006 -5.001 -5.033 -0.033

NaHCO3 1.478e-008 1.480e-008 -7.830 -7.830 0.000

NaSO4- 3.631e-009 3.366e-009 -8.440 -8.473 -0.033

NaCO3- 1.302e-009 1.207e-009 -8.885 -8.918 -0.033

NaOH 3.064e-012 3.068e-012 -11.514 -11.513 0.000

O(0) 3.132e-004

O2 1.566e-004 1.568e-004 -3.805 -3.805 0.000

S(6) 1.154e-004

SO4-2 9.719e-005 7.218e-005 -4.012 -4.142 -0.129

CaSO4 1.180e-005 1.181e-005 -4.928 -4.928 0.000

MgSO4 6.373e-006 6.381e-006 -5.196 -5.195 0.000

NaSO4- 3.631e-009 3.366e-009 -8.440 -8.473 -0.033

KSO4- 1.704e-009 1.580e-009 -8.769 -8.801 -0.033

HSO4- 1.533e-010 1.421e-010 -9.815 -9.847 -0.033

CaHSO4+ 1.502e-012 1.393e-012 -11.823 -11.856 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.87 -7.23 -4.36 CaSO4

Aragonite 0.08 -8.26 -8.34 CaCO3

Calcite 0.23 -8.26 -8.48 CaCO3

CO2(g) -2.42 -3.90 -1.48 CO2

Dolomite 0.25 -16.86 -17.11 CaMg(CO3)2

Gypsum -2.65 -7.23 -4.58 CaSO4:2H2O

H2(g) -23.40 -26.55 -3.15 H2

H2O(g) -1.49 -0.00 1.49 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -0.91 -3.80 -2.90 O2

Initial solution 58. 30/8/2012 02:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.145e-003 3.145e-003

Ca 1.149e-003 1.149e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 2.782e-004 2.782e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.660

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 317

Density (g/cm3) = 0.99711

Activity of water = 1.000

Ionic strength = 4.985e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.264e-003

Total CO2 (mol/kg) = 3.264e-003

Temperature (deg C) = 25.610

Electrical balance (eq) = -8.596e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.31

Iterations = 7

Total H = 1.110155e+002

Total O = 5.551661e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8455 0.7614

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 5.172e-007 4.791e-007 -6.286 -6.320 -0.033

H+ 2.343e-008 2.188e-008 -7.630 -7.660 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.264e-003

HCO3- 3.061e-003 2.844e-003 -2.514 -2.546 -0.032

CO2 1.387e-004 1.389e-004 -3.858 -3.857 0.000

CaHCO3+ 3.215e-005 2.987e-005 -4.493 -4.525 -0.032

MgHCO3+ 1.334e-005 1.237e-005 -4.875 -4.908 -0.033

CaCO3 8.552e-006 8.562e-006 -5.068 -5.067 0.000

CO3-2 8.285e-006 6.170e-006 -5.082 -5.210 -0.128

MgCO3 2.201e-006 2.204e-006 -5.657 -5.657 0.000

NaHCO3 1.480e-008 1.482e-008 -7.830 -7.829 0.000

NaCO3- 1.184e-009 1.098e-009 -8.927 -8.959 -0.033

Ca 1.149e-003

Ca+2 1.096e-003 8.158e-004 -2.960 -3.088 -0.128

CaHCO3+ 3.215e-005 2.987e-005 -4.493 -4.525 -0.032

CaSO4 1.180e-005 1.182e-005 -4.928 -4.927 0.000

CaCO3 8.552e-006 8.562e-006 -5.068 -5.067 0.000

CaOH+ 6.675e-009 6.188e-009 -8.176 -8.208 -0.033

CaHSO4+ 1.646e-012 1.526e-012 -11.784 -11.816 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.306e-005 -4.242 -4.275 -0.033

H(0) 6.728e-027

H2 3.364e-027 3.368e-027 -26.473 -26.473 0.000

K 3.326e-006

K+ 3.324e-006 3.079e-006 -5.478 -5.512 -0.033

KSO4- 1.702e-009 1.578e-009 -8.769 -8.802 -0.033

KOH 4.874e-013 4.880e-013 -12.312 -12.312 0.000

Mg 5.184e-004

Mg+2 4.964e-004 3.708e-004 -3.304 -3.431 -0.127

MgHCO3+ 1.334e-005 1.237e-005 -4.875 -4.908 -0.033

MgSO4 6.366e-006 6.374e-006 -5.196 -5.196 0.000

MgCO3 2.201e-006 2.204e-006 -5.657 -5.657 0.000

MgOH+ 7.012e-008 6.501e-008 -7.154 -7.187 -0.033

Na 1.001e-005

Na+ 9.988e-006 9.266e-006 -5.001 -5.033 -0.033

NaHCO3 1.480e-008 1.482e-008 -7.830 -7.829 0.000

NaSO4- 3.630e-009 3.365e-009 -8.440 -8.473 -0.033

NaCO3- 1.184e-009 1.098e-009 -8.927 -8.959 -0.033

NaOH 2.795e-012 2.798e-012 -11.554 -11.553 0.000

O(0) 2.782e-004

O2 1.391e-004 1.393e-004 -3.857 -3.856 0.000

S(6) 1.154e-004

SO4-2 9.720e-005 7.218e-005 -4.012 -4.142 -0.129

CaSO4 1.180e-005 1.182e-005 -4.928 -4.927 0.000

MgSO4 6.366e-006 6.374e-006 -5.196 -5.196 0.000

NaSO4- 3.630e-009 3.365e-009 -8.440 -8.473 -0.033

KSO4- 1.702e-009 1.578e-009 -8.769 -8.802 -0.033

HSO4- 1.678e-010 1.556e-010 -9.775 -9.808 -0.033

CaHSO4+ 1.646e-012 1.526e-012 -11.784 -11.816 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.87 -7.23 -4.36 CaSO4

Aragonite 0.04 -8.30 -8.34 CaCO3

Calcite 0.19 -8.30 -8.48 CaCO3

CO2(g) -2.38 -3.86 -1.48 CO2

Dolomite 0.17 -16.94 -17.10 CaMg(CO3)2

Gypsum -2.65 -7.23 -4.58 CaSO4:2H2O

H2(g) -23.32 -26.47 -3.15 H2

H2O(g) -1.49 -0.00 1.49 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -0.96 -3.86 -2.90 O2

Initial solution 59. 30/8/2012 02:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.166e-003 3.166e-003

Ca 1.156e-003 1.156e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 2.651e-004 2.651e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.650

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 318

Density (g/cm3) = 0.99712

Activity of water = 1.000

Ionic strength = 5.009e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.289e-003

Total CO2 (mol/kg) = 3.289e-003

Temperature (deg C) = 25.570

Electrical balance (eq) = -9.148e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.38

Iterations = 7

Total H = 1.110156e+002

Total O = 5.551667e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8536 0.7618

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 5.040e-007 4.668e-007 -6.298 -6.331 -0.033

H+ 2.398e-008 2.239e-008 -7.620 -7.650 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.289e-003

HCO3- 3.082e-003 2.862e-003 -2.511 -2.543 -0.032

CO2 1.429e-004 1.431e-004 -3.845 -3.844 0.001

CaHCO3+ 3.254e-005 3.023e-005 -4.488 -4.520 -0.032

MgHCO3+ 1.342e-005 1.244e-005 -4.872 -4.905 -0.033

CaCO3 8.448e-006 8.458e-006 -5.073 -5.073 0.001

CO3-2 8.148e-006 6.065e-006 -5.089 -5.217 -0.128

MgCO3 2.161e-006 2.163e-006 -5.665 -5.665 0.001

NaHCO3 1.489e-008 1.491e-008 -7.827 -7.826 0.001

NaCO3- 1.162e-009 1.077e-009 -8.935 -8.968 -0.033

Ca 1.156e-003

Ca+2 1.103e-003 8.207e-004 -2.957 -3.086 -0.128

CaHCO3+ 3.254e-005 3.023e-005 -4.488 -4.520 -0.032

CaSO4 1.186e-005 1.187e-005 -4.926 -4.926 0.001

CaCO3 8.448e-006 8.458e-006 -5.073 -5.073 0.001

CaOH+ 6.562e-009 6.083e-009 -8.183 -8.216 -0.033

CaHSO4+ 1.691e-012 1.568e-012 -11.772 -11.805 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.305e-005 -4.242 -4.275 -0.033

H(0) 7.048e-027

H2 3.524e-027 3.528e-027 -26.453 -26.452 0.001

K 3.326e-006

K+ 3.324e-006 3.079e-006 -5.478 -5.512 -0.033

KSO4- 1.699e-009 1.575e-009 -8.770 -8.803 -0.033

KOH 4.762e-013 4.768e-013 -12.322 -12.322 0.001

Mg 5.184e-004

Mg+2 4.964e-004 3.706e-004 -3.304 -3.431 -0.127

MgHCO3+ 1.342e-005 1.244e-005 -4.872 -4.905 -0.033

MgSO4 6.349e-006 6.357e-006 -5.197 -5.197 0.001

MgCO3 2.161e-006 2.163e-006 -5.665 -5.665 0.001

MgOH+ 6.825e-008 6.326e-008 -7.166 -7.199 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.264e-006 -5.001 -5.033 -0.033

NaHCO3 1.489e-008 1.491e-008 -7.827 -7.826 0.001

NaSO4- 3.625e-009 3.360e-009 -8.441 -8.474 -0.033

NaCO3- 1.162e-009 1.077e-009 -8.935 -8.968 -0.033

NaOH 2.731e-012 2.734e-012 -11.564 -11.563 0.001

O(0) 2.651e-004

O2 1.325e-004 1.327e-004 -3.878 -3.877 0.001

S(6) 1.154e-004

SO4-2 9.716e-005 7.211e-005 -4.013 -4.142 -0.129

CaSO4 1.186e-005 1.187e-005 -4.926 -4.926 0.001

MgSO4 6.349e-006 6.357e-006 -5.197 -5.197 0.001

NaSO4- 3.625e-009 3.360e-009 -8.441 -8.474 -0.033

KSO4- 1.699e-009 1.575e-009 -8.770 -8.803 -0.033

HSO4- 1.714e-010 1.589e-010 -9.766 -9.799 -0.033

CaHSO4+ 1.691e-012 1.568e-012 -11.772 -11.805 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.86 -7.23 -4.36 CaSO4

Aragonite 0.04 -8.30 -8.34 CaCO3

Calcite 0.18 -8.30 -8.48 CaCO3

CO2(g) -2.37 -3.84 -1.47 CO2

Dolomite 0.15 -16.95 -17.10 CaMg(CO3)2

Gypsum -2.65 -7.23 -4.58 CaSO4:2H2O

H2(g) -23.30 -26.45 -3.15 H2

H2O(g) -1.50 -0.00 1.50 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -0.98 -3.88 -2.90 O2

Initial solution 60. 30/8/2012 02:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.176e-003 3.176e-003

Ca 1.160e-003 1.160e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 2.357e-004 2.357e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.630

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 318

Density (g/cm3) = 0.99714

Activity of water = 1.000

Ionic strength = 5.022e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.308e-003

Total CO2 (mol/kg) = 3.308e-003

Temperature (deg C) = 25.480

Electrical balance (eq) = -9.448e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.43

Iterations = 7

Total H = 1.110156e+002

Total O = 5.551669e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8683 0.7625

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 4.781e-007 4.428e-007 -6.320 -6.354 -0.033

H+ 2.511e-008 2.344e-008 -7.600 -7.630 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.308e-003

HCO3- 3.093e-003 2.873e-003 -2.510 -2.542 -0.032

CO2 1.504e-004 1.506e-004 -3.823 -3.822 0.001

CaHCO3+ 3.273e-005 3.040e-005 -4.485 -4.517 -0.032

MgHCO3+ 1.347e-005 1.248e-005 -4.871 -4.904 -0.033

CaCO3 8.095e-006 8.105e-006 -5.092 -5.091 0.001

CO3-2 7.799e-006 5.803e-006 -5.108 -5.236 -0.128

MgCO3 2.065e-006 2.067e-006 -5.685 -5.685 0.001

NaHCO3 1.495e-008 1.497e-008 -7.825 -7.825 0.001

NaCO3- 1.106e-009 1.026e-009 -8.956 -8.989 -0.033

Ca 1.160e-003

Ca+2 1.107e-003 8.233e-004 -2.956 -3.084 -0.129

CaHCO3+ 3.273e-005 3.040e-005 -4.485 -4.517 -0.032

CaSO4 1.188e-005 1.189e-005 -4.925 -4.925 0.001

CaCO3 8.095e-006 8.105e-006 -5.092 -5.091 0.001

CaOH+ 6.288e-009 5.828e-009 -8.202 -8.234 -0.033

CaHSO4+ 1.773e-012 1.643e-012 -11.751 -11.784 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.304e-005 -4.242 -4.275 -0.033

H(0) 7.735e-027

H2 3.867e-027 3.872e-027 -26.413 -26.412 0.001

K 3.326e-006

K+ 3.324e-006 3.078e-006 -5.478 -5.512 -0.033

KSO4- 1.696e-009 1.572e-009 -8.771 -8.803 -0.033

KOH 4.547e-013 4.553e-013 -12.342 -12.342 0.001

Mg 5.184e-004

Mg+2 4.965e-004 3.705e-004 -3.304 -3.431 -0.127

MgHCO3+ 1.347e-005 1.248e-005 -4.871 -4.904 -0.033

MgSO4 6.331e-006 6.339e-006 -5.199 -5.198 0.001

MgCO3 2.065e-006 2.067e-006 -5.685 -5.685 0.001

MgOH+ 6.464e-008 5.992e-008 -7.189 -7.222 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.264e-006 -5.001 -5.033 -0.033

NaHCO3 1.495e-008 1.497e-008 -7.825 -7.825 0.001

NaSO4- 3.622e-009 3.357e-009 -8.441 -8.474 -0.033

NaCO3- 1.106e-009 1.026e-009 -8.956 -8.989 -0.033

NaOH 2.608e-012 2.611e-012 -11.584 -11.583 0.001

O(0) 2.357e-004

O2 1.178e-004 1.180e-004 -3.929 -3.928 0.001

S(6) 1.154e-004

SO4-2 9.715e-005 7.208e-005 -4.013 -4.142 -0.130

CaSO4 1.188e-005 1.189e-005 -4.925 -4.925 0.001

MgSO4 6.331e-006 6.339e-006 -5.199 -5.198 0.001

NaSO4- 3.622e-009 3.357e-009 -8.441 -8.474 -0.033

KSO4- 1.696e-009 1.572e-009 -8.771 -8.803 -0.033

HSO4- 1.791e-010 1.660e-010 -9.747 -9.780 -0.033

CaHSO4+ 1.773e-012 1.643e-012 -11.751 -11.784 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.86 -7.23 -4.36 CaSO4

Aragonite 0.02 -8.32 -8.34 CaCO3

Calcite 0.16 -8.32 -8.48 CaCO3

CO2(g) -2.35 -3.82 -1.47 CO2

Dolomite 0.11 -16.99 -17.10 CaMg(CO3)2

Gypsum -2.65 -7.23 -4.58 CaSO4:2H2O

H2(g) -23.26 -26.41 -3.15 H2

H2O(g) -1.50 -0.00 1.50 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -1.03 -3.93 -2.90 O2

Initial solution 61. 30/8/2012 02:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.197e-003 3.197e-003

Ca 1.167e-003 1.167e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 2.244e-004 2.244e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.610

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 319

Density (g/cm3) = 0.99716

Activity of water = 1.000

Ionic strength = 5.047e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.337e-003

Total CO2 (mol/kg) = 3.337e-003

Temperature (deg C) = 25.410

Electrical balance (eq) = -1.000e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.50

Iterations = 7

Total H = 1.110156e+002

Total O = 5.551676e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8887 0.7635

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 4.543e-007 4.206e-007 -6.343 -6.376 -0.033

H+ 2.630e-008 2.455e-008 -7.580 -7.610 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.337e-003

HCO3- 3.115e-003 2.893e-003 -2.507 -2.539 -0.032

CO2 1.587e-004 1.589e-004 -3.799 -3.799 0.001

CaHCO3+ 3.312e-005 3.076e-005 -4.480 -4.512 -0.032

MgHCO3+ 1.355e-005 1.256e-005 -4.868 -4.901 -0.033

CaCO3 7.808e-006 7.817e-006 -5.107 -5.107 0.001

CO3-2 7.492e-006 5.572e-006 -5.125 -5.254 -0.129

MgCO3 1.979e-006 1.981e-006 -5.704 -5.703 0.001

NaHCO3 1.505e-008 1.507e-008 -7.823 -7.822 0.001

NaCO3- 1.059e-009 9.810e-010 -8.975 -9.008 -0.033

Ca 1.167e-003

Ca+2 1.114e-003 8.282e-004 -2.953 -3.082 -0.129

CaHCO3+ 3.312e-005 3.076e-005 -4.480 -4.512 -0.032

CaSO4 1.193e-005 1.195e-005 -4.923 -4.923 0.001

CaCO3 7.808e-006 7.817e-006 -5.107 -5.107 0.001

CaOH+ 6.042e-009 5.599e-009 -8.219 -8.252 -0.033

CaHSO4+ 1.863e-012 1.727e-012 -11.730 -11.763 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.303e-005 -4.242 -4.275 -0.033

H(0) 8.487e-027

H2 4.244e-027 4.248e-027 -26.372 -26.372 0.001

K 3.326e-006

K+ 3.324e-006 3.078e-006 -5.478 -5.512 -0.033

KSO4- 1.692e-009 1.569e-009 -8.771 -8.805 -0.033

KOH 4.342e-013 4.347e-013 -12.362 -12.362 0.001

Mg 5.184e-004

Mg+2 4.965e-004 3.703e-004 -3.304 -3.431 -0.127

MgHCO3+ 1.355e-005 1.256e-005 -4.868 -4.901 -0.033

MgSO4 6.310e-006 6.318e-006 -5.200 -5.199 0.001

MgCO3 1.979e-006 1.981e-006 -5.704 -5.703 0.001

MgOH+ 6.132e-008 5.683e-008 -7.212 -7.245 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.262e-006 -5.001 -5.033 -0.033

NaHCO3 1.505e-008 1.507e-008 -7.823 -7.822 0.001

NaSO4- 3.617e-009 3.352e-009 -8.442 -8.475 -0.033

NaCO3- 1.059e-009 9.810e-010 -8.975 -9.008 -0.033

NaOH 2.490e-012 2.493e-012 -11.604 -11.603 0.001

O(0) 2.244e-004

O2 1.122e-004 1.123e-004 -3.950 -3.949 0.001

S(6) 1.154e-004

SO4-2 9.712e-005 7.201e-005 -4.013 -4.143 -0.130

CaSO4 1.193e-005 1.195e-005 -4.923 -4.923 0.001

MgSO4 6.310e-006 6.318e-006 -5.200 -5.199 0.001

NaSO4- 3.617e-009 3.352e-009 -8.442 -8.475 -0.033

KSO4- 1.692e-009 1.569e-009 -8.771 -8.805 -0.033

HSO4- 1.871e-010 1.734e-010 -9.728 -9.761 -0.033

CaHSO4+ 1.863e-012 1.727e-012 -11.730 -11.763 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.86 -7.22 -4.36 CaSO4

Aragonite 0.00 -8.34 -8.34 CaCO3

Calcite 0.15 -8.34 -8.48 CaCO3

CO2(g) -2.33 -3.80 -1.47 CO2

Dolomite 0.08 -17.02 -17.10 CaMg(CO3)2

Gypsum -2.64 -7.22 -4.58 CaSO4:2H2O

H2(g) -23.22 -26.37 -3.15 H2

H2O(g) -1.50 -0.00 1.50 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -1.05 -3.95 -2.90 O2

Initial solution 62. 30/8/2012 03:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.207e-003 3.207e-003

Ca 1.171e-003 1.171e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.913e-004 1.913e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.590

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 320

Density (g/cm3) = 0.99717

Activity of water = 1.000

Ionic strength = 5.060e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.357e-003

Total CO2 (mol/kg) = 3.357e-003

Temperature (deg C) = 25.380

Electrical balance (eq) = -1.028e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.54

Iterations = 7

Total H = 1.110156e+002

Total O = 5.551677e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8939 0.7637

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 4.329e-007 4.008e-007 -6.364 -6.397 -0.034

H+ 2.754e-008 2.570e-008 -7.560 -7.590 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.357e-003

HCO3- 3.126e-003 2.903e-003 -2.505 -2.537 -0.032

CO2 1.668e-004 1.670e-004 -3.778 -3.777 0.001

CaHCO3+ 3.333e-005 3.095e-005 -4.477 -4.509 -0.032

MgHCO3+ 1.359e-005 1.260e-005 -4.867 -4.900 -0.033

CaCO3 7.498e-006 7.506e-006 -5.125 -5.125 0.001

CO3-2 7.179e-006 5.337e-006 -5.144 -5.273 -0.129

MgCO3 1.894e-006 1.897e-006 -5.723 -5.722 0.001

NaHCO3 1.510e-008 1.512e-008 -7.821 -7.820 0.001

NaCO3- 1.012e-009 9.382e-010 -8.995 -9.028 -0.033

Ca 1.171e-003

Ca+2 1.118e-003 8.308e-004 -2.951 -3.080 -0.129

CaHCO3+ 3.333e-005 3.095e-005 -4.477 -4.509 -0.032

CaSO4 1.196e-005 1.197e-005 -4.922 -4.922 0.001

CaCO3 7.498e-006 7.506e-006 -5.125 -5.125 0.001

CaOH+ 5.788e-009 5.364e-009 -8.237 -8.271 -0.033

CaHSO4+ 1.955e-012 1.812e-012 -11.709 -11.742 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.303e-005 -4.242 -4.275 -0.033

H(0) 9.309e-027

H2 4.654e-027 4.660e-027 -26.332 -26.332 0.001

K 3.326e-006

K+ 3.324e-006 3.078e-006 -5.478 -5.512 -0.033

KSO4- 1.691e-009 1.567e-009 -8.772 -8.805 -0.033

KOH 4.146e-013 4.151e-013 -12.382 -12.382 0.001

Mg 5.184e-004

Mg+2 4.966e-004 3.702e-004 -3.304 -3.432 -0.127

MgHCO3+ 1.359e-005 1.260e-005 -4.867 -4.900 -0.033

MgSO4 6.301e-006 6.308e-006 -5.201 -5.200 0.001

MgCO3 1.894e-006 1.897e-006 -5.723 -5.722 0.001

MgOH+ 5.840e-008 5.412e-008 -7.234 -7.267 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.261e-006 -5.001 -5.033 -0.033

NaHCO3 1.510e-008 1.512e-008 -7.821 -7.820 0.001

NaSO4- 3.614e-009 3.349e-009 -8.442 -8.475 -0.033

NaCO3- 1.012e-009 9.382e-010 -8.995 -9.028 -0.033

NaOH 2.378e-012 2.380e-012 -11.624 -11.623 0.001

O(0) 1.913e-004

O2 9.565e-005 9.576e-005 -4.019 -4.019 0.001

S(6) 1.154e-004

SO4-2 9.710e-005 7.198e-005 -4.013 -4.143 -0.130

CaSO4 1.196e-005 1.197e-005 -4.922 -4.922 0.001

MgSO4 6.301e-006 6.308e-006 -5.201 -5.200 0.001

NaSO4- 3.614e-009 3.349e-009 -8.442 -8.475 -0.033

KSO4- 1.691e-009 1.567e-009 -8.772 -8.805 -0.033

HSO4- 1.957e-010 1.814e-010 -9.708 -9.741 -0.033

CaHSO4+ 1.955e-012 1.812e-012 -11.709 -11.742 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.86 -7.22 -4.36 CaSO4

Aragonite -0.01 -8.35 -8.34 CaCO3

Calcite 0.13 -8.35 -8.48 CaCO3

CO2(g) -2.30 -3.78 -1.47 CO2

Dolomite 0.04 -17.06 -17.10 CaMg(CO3)2

Gypsum -2.64 -7.22 -4.58 CaSO4:2H2O

H2(g) -23.18 -26.33 -3.15 H2

H2O(g) -1.50 -0.00 1.50 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -1.12 -4.02 -2.90 O2

Initial solution 63. 30/8/2012 03:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.217e-003 3.217e-003

Ca 1.175e-003 1.175e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.700e-004 1.700e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.560

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 320

Density (g/cm3) = 0.99718

Activity of water = 1.000

Ionic strength = 5.074e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.381e-003

Total CO2 (mol/kg) = 3.381e-003

Temperature (deg C) = 25.330

Electrical balance (eq) = -1.058e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.58

Iterations = 6

Total H = 1.110156e+002

Total O = 5.551681e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.9152 0.7649

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 4.025e-007 3.726e-007 -6.395 -6.429 -0.034

H+ 2.951e-008 2.754e-008 -7.530 -7.560 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.381e-003

HCO3- 3.139e-003 2.914e-003 -2.503 -2.535 -0.032

CO2 1.795e-004 1.798e-004 -3.746 -3.745 0.001

CaHCO3+ 3.354e-005 3.115e-005 -4.474 -4.507 -0.032

MgHCO3+ 1.364e-005 1.264e-005 -4.865 -4.898 -0.033

CaCO3 7.033e-006 7.041e-006 -5.153 -5.152 0.001

CO3-2 6.721e-006 4.995e-006 -5.173 -5.301 -0.129

MgCO3 1.771e-006 1.773e-006 -5.752 -5.751 0.001

NaHCO3 1.516e-008 1.518e-008 -7.819 -7.819 0.001

NaCO3- 9.452e-010 8.758e-010 -9.024 -9.058 -0.033

Ca 1.175e-003

Ca+2 1.122e-003 8.335e-004 -2.950 -3.079 -0.129

CaHCO3+ 3.354e-005 3.115e-005 -4.474 -4.507 -0.032

CaSO4 1.199e-005 1.200e-005 -4.921 -4.921 0.001

CaCO3 7.033e-006 7.041e-006 -5.153 -5.152 0.001

CaOH+ 5.420e-009 5.022e-009 -8.266 -8.299 -0.033

CaHSO4+ 2.098e-012 1.944e-012 -11.678 -11.711 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.303e-005 -4.242 -4.276 -0.033

H(0) 1.069e-026

H2 5.346e-027 5.353e-027 -26.272 -26.271 0.001

K 3.326e-006

K+ 3.324e-006 3.077e-006 -5.478 -5.512 -0.033

KSO4- 1.688e-009 1.565e-009 -8.773 -8.806 -0.033

KOH 3.869e-013 3.874e-013 -12.412 -12.412 0.001

Mg 5.184e-004

Mg+2 4.966e-004 3.702e-004 -3.304 -3.432 -0.128

MgHCO3+ 1.364e-005 1.264e-005 -4.865 -4.898 -0.033

MgSO4 6.289e-006 6.296e-006 -5.201 -5.201 0.001

MgCO3 1.771e-006 1.773e-006 -5.752 -5.751 0.001

MgOH+ 5.425e-008 5.027e-008 -7.266 -7.299 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.261e-006 -5.001 -5.033 -0.033

NaHCO3 1.516e-008 1.518e-008 -7.819 -7.819 0.001

NaSO4- 3.611e-009 3.346e-009 -8.442 -8.475 -0.033

NaCO3- 9.452e-010 8.758e-010 -9.024 -9.058 -0.033

NaOH 2.219e-012 2.221e-012 -11.654 -11.653 0.001

O(0) 1.700e-004

O2 8.502e-005 8.512e-005 -4.070 -4.070 0.001

S(6) 1.154e-004

SO4-2 9.709e-005 7.194e-005 -4.013 -4.143 -0.130

CaSO4 1.199e-005 1.200e-005 -4.921 -4.921 0.001

MgSO4 6.289e-006 6.296e-006 -5.201 -5.201 0.001

NaSO4- 3.611e-009 3.346e-009 -8.442 -8.475 -0.033

KSO4- 1.688e-009 1.565e-009 -8.773 -8.806 -0.033

HSO4- 2.094e-010 1.940e-010 -9.679 -9.712 -0.033

CaHSO4+ 2.098e-012 1.944e-012 -11.678 -11.711 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.86 -7.22 -4.36 CaSO4

Aragonite -0.04 -8.38 -8.34 CaCO3

Calcite 0.10 -8.38 -8.48 CaCO3

CO2(g) -2.27 -3.75 -1.47 CO2

Dolomite -0.02 -17.11 -17.10 CaMg(CO3)2

Gypsum -2.64 -7.22 -4.58 CaSO4:2H2O

H2(g) -23.12 -26.27 -3.15 H2

H2O(g) -1.50 -0.00 1.50 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -1.18 -4.07 -2.89 O2

Initial solution 64. 30/8/2012 03:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.228e-003 3.228e-003

Ca 1.178e-003 1.178e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.457e-004 1.457e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.550

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 321

Density (g/cm3) = 0.99720

Activity of water = 1.000

Ionic strength = 5.086e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.396e-003

Total CO2 (mol/kg) = 3.396e-003

Temperature (deg C) = 25.260

Electrical balance (eq) = -1.085e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.61

Iterations = 6

Total H = 1.110156e+002

Total O = 5.551683e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.9142 0.7646

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.913e-007 3.622e-007 -6.407 -6.441 -0.034

H+ 3.020e-008 2.818e-008 -7.520 -7.550 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.396e-003

HCO3- 3.149e-003 2.924e-003 -2.502 -2.534 -0.032

CO2 1.845e-004 1.847e-004 -3.734 -3.734 0.001

CaHCO3+ 3.372e-005 3.131e-005 -4.472 -4.504 -0.032

MgHCO3+ 1.368e-005 1.268e-005 -4.864 -4.897 -0.033

CaCO3 6.896e-006 6.904e-006 -5.161 -5.161 0.001

CO3-2 6.583e-006 4.891e-006 -5.182 -5.311 -0.129

MgCO3 1.732e-006 1.734e-006 -5.761 -5.761 0.001

NaHCO3 1.521e-008 1.523e-008 -7.818 -7.817 0.001

NaCO3- 9.222e-010 8.544e-010 -9.035 -9.068 -0.033

Ca 1.178e-003

Ca+2 1.126e-003 8.360e-004 -2.949 -3.078 -0.129

CaHCO3+ 3.372e-005 3.131e-005 -4.472 -4.504 -0.032

CaSO4 1.201e-005 1.202e-005 -4.920 -4.920 0.001

CaCO3 6.896e-006 6.904e-006 -5.161 -5.161 0.001

CaOH+ 5.312e-009 4.922e-009 -8.275 -8.308 -0.033

CaHSO4+ 2.150e-012 1.992e-012 -11.668 -11.701 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.302e-005 -4.242 -4.276 -0.034

H(0) 1.120e-026

H2 5.602e-027 5.609e-027 -26.252 -26.251 0.001

K 3.326e-006

K+ 3.324e-006 3.077e-006 -5.478 -5.512 -0.034

KSO4- 1.686e-009 1.562e-009 -8.773 -8.806 -0.033

KOH 3.781e-013 3.785e-013 -12.422 -12.422 0.001

Mg 5.184e-004

Mg+2 4.967e-004 3.701e-004 -3.304 -3.432 -0.128

MgHCO3+ 1.368e-005 1.268e-005 -4.864 -4.897 -0.033

MgSO4 6.274e-006 6.281e-006 -5.202 -5.202 0.001

MgCO3 1.732e-006 1.734e-006 -5.761 -5.761 0.001

MgOH+ 5.267e-008 4.880e-008 -7.278 -7.312 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.260e-006 -5.001 -5.033 -0.033

NaHCO3 1.521e-008 1.523e-008 -7.818 -7.817 0.001

NaSO4- 3.608e-009 3.343e-009 -8.443 -8.476 -0.033

NaCO3- 9.222e-010 8.544e-010 -9.035 -9.068 -0.033

NaOH 2.168e-012 2.171e-012 -11.664 -11.663 0.001

O(0) 1.457e-004

O2 7.283e-005 7.292e-005 -4.138 -4.137 0.001

S(6) 1.154e-004

SO4-2 9.708e-005 7.191e-005 -4.013 -4.143 -0.130

CaSO4 1.201e-005 1.202e-005 -4.920 -4.920 0.001

MgSO4 6.274e-006 6.281e-006 -5.202 -5.202 0.001

NaSO4- 3.608e-009 3.343e-009 -8.443 -8.476 -0.033

KSO4- 1.686e-009 1.562e-009 -8.773 -8.806 -0.033

HSO4- 2.139e-010 1.982e-010 -9.670 -9.703 -0.033

CaHSO4+ 2.150e-012 1.992e-012 -11.668 -11.701 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.86 -7.22 -4.36 CaSO4

Aragonite -0.05 -8.39 -8.34 CaCO3

Calcite 0.09 -8.39 -8.48 CaCO3

CO2(g) -2.26 -3.73 -1.47 CO2

Dolomite -0.03 -17.13 -17.10 CaMg(CO3)2

Gypsum -2.64 -7.22 -4.58 CaSO4:2H2O

H2(g) -23.10 -26.25 -3.15 H2

H2O(g) -1.50 -0.00 1.50 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -1.24 -4.14 -2.89 O2

Initial solution 65. 30/8/2012 03:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.248e-003 3.248e-003

Ca 1.186e-003 1.186e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.300e-004 1.300e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.550

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 322

Density (g/cm3) = 0.99722

Activity of water = 1.000

Ionic strength = 5.110e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.418e-003

Total CO2 (mol/kg) = 3.418e-003

Temperature (deg C) = 25.200

Electrical balance (eq) = -1.144e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.69

Iterations = 6

Total H = 1.110157e+002

Total O = 5.551688e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.9068 0.7640

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.896e-007 3.606e-007 -6.409 -6.443 -0.034

H+ 3.020e-008 2.818e-008 -7.520 -7.550 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.418e-003

HCO3- 3.169e-003 2.942e-003 -2.499 -2.531 -0.032

CO2 1.858e-004 1.860e-004 -3.731 -3.730 0.001

CaHCO3+ 3.410e-005 3.165e-005 -4.467 -4.500 -0.032

MgHCO3+ 1.376e-005 1.274e-005 -4.862 -4.895 -0.033

CaCO3 6.961e-006 6.970e-006 -5.157 -5.157 0.001

CO3-2 6.620e-006 4.915e-006 -5.179 -5.308 -0.129

MgCO3 1.738e-006 1.740e-006 -5.760 -5.759 0.001

NaHCO3 1.530e-008 1.532e-008 -7.815 -7.815 0.001

NaCO3- 9.240e-010 8.560e-010 -9.034 -9.068 -0.033

Ca 1.186e-003

Ca+2 1.133e-003 8.407e-004 -2.946 -3.075 -0.130

CaHCO3+ 3.410e-005 3.165e-005 -4.467 -4.500 -0.032

CaSO4 1.206e-005 1.207e-005 -4.919 -4.918 0.001

CaCO3 6.961e-006 6.970e-006 -5.157 -5.157 0.001

CaOH+ 5.343e-009 4.950e-009 -8.272 -8.305 -0.033

CaHSO4+ 2.157e-012 1.999e-012 -11.666 -11.699 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.301e-005 -4.242 -4.276 -0.034

H(0) 1.121e-026

H2 5.606e-027 5.612e-027 -26.251 -26.251 0.001

K 3.326e-006

K+ 3.324e-006 3.077e-006 -5.478 -5.512 -0.034

KSO4- 1.682e-009 1.559e-009 -8.774 -8.807 -0.033

KOH 3.780e-013 3.785e-013 -12.422 -12.422 0.001

Mg 5.184e-004

Mg+2 4.966e-004 3.698e-004 -3.304 -3.432 -0.128

MgHCO3+ 1.376e-005 1.274e-005 -4.862 -4.895 -0.033

MgSO4 6.254e-006 6.261e-006 -5.204 -5.203 0.001

MgCO3 1.738e-006 1.740e-006 -5.760 -5.759 0.001

MgOH+ 5.236e-008 4.851e-008 -7.281 -7.314 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.258e-006 -5.001 -5.033 -0.033

NaHCO3 1.530e-008 1.532e-008 -7.815 -7.815 0.001

NaSO4- 3.603e-009 3.338e-009 -8.443 -8.476 -0.033

NaCO3- 9.240e-010 8.560e-010 -9.034 -9.068 -0.033

NaOH 2.168e-012 2.170e-012 -11.664 -11.664 0.001

O(0) 1.300e-004

O2 6.502e-005 6.509e-005 -4.187 -4.186 0.001

S(6) 1.154e-004

SO4-2 9.705e-005 7.185e-005 -4.013 -4.144 -0.131

CaSO4 1.206e-005 1.207e-005 -4.919 -4.918 0.001

MgSO4 6.254e-006 6.261e-006 -5.204 -5.203 0.001

NaSO4- 3.603e-009 3.338e-009 -8.443 -8.476 -0.033

KSO4- 1.682e-009 1.559e-009 -8.774 -8.807 -0.033

HSO4- 2.135e-010 1.977e-010 -9.671 -9.704 -0.033

CaHSO4+ 2.157e-012 1.999e-012 -11.666 -11.699 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.86 -7.22 -4.36 CaSO4

Aragonite -0.05 -8.38 -8.34 CaCO3

Calcite 0.10 -8.38 -8.48 CaCO3

CO2(g) -2.26 -3.73 -1.47 CO2

Dolomite -0.03 -17.12 -17.09 CaMg(CO3)2

Gypsum -2.64 -7.22 -4.58 CaSO4:2H2O

H2(g) -23.10 -26.25 -3.15 H2

H2O(g) -1.50 -0.00 1.50 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -1.29 -4.19 -2.89 O2

Initial solution 66. 30/8/2012 04:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.259e-003 3.259e-003

Ca 1.190e-003 1.190e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.069e-004 1.069e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.530

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 322

Density (g/cm3) = 0.99724

Activity of water = 1.000

Ionic strength = 5.123e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.439e-003

Total CO2 (mol/kg) = 3.439e-003

Temperature (deg C) = 25.130

Electrical balance (eq) = -1.170e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.73

Iterations = 6

Total H = 1.110157e+002

Total O = 5.551691e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.9114 0.7641

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.702e-007 3.425e-007 -6.432 -6.465 -0.034

H+ 3.163e-008 2.951e-008 -7.500 -7.530 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.439e-003

HCO3- 3.181e-003 2.952e-003 -2.497 -2.530 -0.032

CO2 1.954e-004 1.956e-004 -3.709 -3.709 0.001

CaHCO3+ 3.429e-005 3.183e-005 -4.465 -4.497 -0.032

MgHCO3+ 1.380e-005 1.278e-005 -4.860 -4.893 -0.033

CaCO3 6.673e-006 6.681e-006 -5.176 -5.175 0.001

CO3-2 6.337e-006 4.704e-006 -5.198 -5.328 -0.129

MgCO3 1.661e-006 1.663e-006 -5.780 -5.779 0.001

NaHCO3 1.535e-008 1.537e-008 -7.814 -7.813 0.001

NaCO3- 8.811e-010 8.162e-010 -9.055 -9.088 -0.033

Ca 1.190e-003

Ca+2 1.137e-003 8.433e-004 -2.944 -3.074 -0.130

CaHCO3+ 3.429e-005 3.183e-005 -4.465 -4.497 -0.032

CaSO4 1.208e-005 1.210e-005 -4.918 -4.917 0.001

CaCO3 6.673e-006 6.681e-006 -5.176 -5.175 0.001

CaOH+ 5.119e-009 4.742e-009 -8.291 -8.324 -0.033

CaHSO4+ 2.262e-012 2.095e-012 -11.646 -11.679 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.301e-005 -4.242 -4.276 -0.034

H(0) 1.230e-026

H2 6.151e-027 6.158e-027 -26.211 -26.211 0.001

K 3.326e-006

K+ 3.324e-006 3.076e-006 -5.478 -5.512 -0.034

KSO4- 1.680e-009 1.556e-009 -8.775 -8.808 -0.033

KOH 3.610e-013 3.614e-013 -12.443 -12.442 0.001

Mg 5.184e-004

Mg+2 4.967e-004 3.698e-004 -3.304 -3.432 -0.128

MgHCO3+ 1.380e-005 1.278e-005 -4.860 -4.893 -0.033

MgSO4 6.239e-006 6.246e-006 -5.205 -5.204 0.001

MgCO3 1.661e-006 1.663e-006 -5.780 -5.779 0.001

MgOH+ 4.969e-008 4.602e-008 -7.304 -7.337 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.258e-006 -5.001 -5.033 -0.033

NaHCO3 1.535e-008 1.537e-008 -7.814 -7.813 0.001

NaSO4- 3.600e-009 3.335e-009 -8.444 -8.477 -0.033

NaCO3- 8.811e-010 8.162e-010 -9.055 -9.088 -0.033

NaOH 2.070e-012 2.072e-012 -11.684 -11.684 0.001

O(0) 1.069e-004

O2 5.345e-005 5.352e-005 -4.272 -4.272 0.001

S(6) 1.154e-004

SO4-2 9.704e-005 7.182e-005 -4.013 -4.144 -0.131

CaSO4 1.208e-005 1.210e-005 -4.918 -4.917 0.001

MgSO4 6.239e-006 6.246e-006 -5.205 -5.204 0.001

NaSO4- 3.600e-009 3.335e-009 -8.444 -8.477 -0.033

KSO4- 1.680e-009 1.556e-009 -8.775 -8.808 -0.033

HSO4- 2.231e-010 2.067e-010 -9.652 -9.685 -0.033

CaHSO4+ 2.262e-012 2.095e-012 -11.646 -11.679 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.86 -7.22 -4.36 CaSO4

Aragonite -0.06 -8.40 -8.34 CaCO3

Calcite 0.08 -8.40 -8.48 CaCO3

CO2(g) -2.24 -3.71 -1.47 CO2

Dolomite -0.07 -17.16 -17.09 CaMg(CO3)2

Gypsum -2.64 -7.22 -4.58 CaSO4:2H2O

H2(g) -23.06 -26.21 -3.15 H2

H2O(g) -1.51 -0.00 1.51 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -1.38 -4.27 -2.89 O2

Initial solution 67. 30/8/2012 04:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.269e-003 3.269e-003

Ca 1.193e-003 1.193e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 7.189e-005 7.189e-005

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.520

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 322

Density (g/cm3) = 0.99726

Activity of water = 1.000

Ionic strength = 5.136e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.455e-003

Total CO2 (mol/kg) = 3.455e-003

Temperature (deg C) = 25.050

Electrical balance (eq) = -1.199e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.77

Iterations = 6

Total H = 1.110157e+002

Total O = 5.551691e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8849 0.7623

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.596e-007 3.327e-007 -6.444 -6.478 -0.034

H+ 3.237e-008 3.020e-008 -7.490 -7.520 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.455e-003

HCO3- 3.191e-003 2.962e-003 -2.496 -2.528 -0.032

CO2 2.008e-004 2.010e-004 -3.697 -3.697 0.001

CaHCO3+ 3.446e-005 3.199e-005 -4.463 -4.495 -0.032

MgHCO3+ 1.384e-005 1.282e-005 -4.859 -4.892 -0.033

CaCO3 6.541e-006 6.548e-006 -5.184 -5.184 0.001

CO3-2 6.205e-006 4.605e-006 -5.207 -5.337 -0.130

MgCO3 1.624e-006 1.626e-006 -5.790 -5.789 0.001

NaHCO3 1.540e-008 1.542e-008 -7.812 -7.812 0.001

NaCO3- 8.591e-010 7.957e-010 -9.066 -9.099 -0.033

Ca 1.193e-003

Ca+2 1.140e-003 8.457e-004 -2.943 -3.073 -0.130

CaHCO3+ 3.446e-005 3.199e-005 -4.463 -4.495 -0.032

CaSO4 1.211e-005 1.212e-005 -4.917 -4.916 0.001

CaCO3 6.541e-006 6.548e-006 -5.184 -5.184 0.001

CaOH+ 5.017e-009 4.647e-009 -8.300 -8.333 -0.033

CaHSO4+ 2.317e-012 2.146e-012 -11.635 -11.668 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.300e-005 -4.242 -4.276 -0.034

H(0) 1.289e-026

H2 6.446e-027 6.453e-027 -26.191 -26.190 0.001

K 3.326e-006

K+ 3.324e-006 3.076e-006 -5.478 -5.512 -0.034

KSO4- 1.677e-009 1.553e-009 -8.776 -8.809 -0.033

KOH 3.527e-013 3.531e-013 -12.453 -12.452 0.001

Mg 5.184e-004

Mg+2 4.967e-004 3.697e-004 -3.304 -3.432 -0.128

MgHCO3+ 1.384e-005 1.282e-005 -4.859 -4.892 -0.033

MgSO4 6.222e-006 6.230e-006 -5.206 -5.206 0.001

MgCO3 1.624e-006 1.626e-006 -5.790 -5.789 0.001

MgOH+ 4.820e-008 4.464e-008 -7.317 -7.350 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.257e-006 -5.001 -5.034 -0.033

NaHCO3 1.540e-008 1.542e-008 -7.812 -7.812 0.001

NaSO4- 3.597e-009 3.332e-009 -8.444 -8.477 -0.033

NaCO3- 8.591e-010 7.957e-010 -9.066 -9.099 -0.033

NaOH 2.023e-012 2.025e-012 -11.694 -11.694 0.001

O(0) 7.189e-005

O2 3.595e-005 3.599e-005 -4.444 -4.444 0.001

S(6) 1.154e-004

SO4-2 9.704e-005 7.179e-005 -4.013 -4.144 -0.131

CaSO4 1.211e-005 1.212e-005 -4.917 -4.916 0.001

MgSO4 6.222e-006 6.230e-006 -5.206 -5.206 0.001

NaSO4- 3.597e-009 3.332e-009 -8.444 -8.477 -0.033

KSO4- 1.677e-009 1.553e-009 -8.776 -8.809 -0.033

HSO4- 2.278e-010 2.110e-010 -9.642 -9.676 -0.033

CaHSO4+ 2.317e-012 2.146e-012 -11.635 -11.668 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.86 -7.22 -4.36 CaSO4

Aragonite -0.07 -8.41 -8.34 CaCO3

Calcite 0.07 -8.41 -8.48 CaCO3

CO2(g) -2.23 -3.70 -1.47 CO2

Dolomite -0.09 -17.18 -17.09 CaMg(CO3)2

Gypsum -2.64 -7.22 -4.58 CaSO4:2H2O

H2(g) -23.04 -26.19 -3.15 H2

H2O(g) -1.51 -0.00 1.51 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -1.55 -4.44 -2.89 O2

Initial solution 68. 30/8/2012 04:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.269e-003 3.269e-003

Ca 1.193e-003 1.193e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.001e-005 4.001e-005

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.500

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 322

Density (g/cm3) = 0.99727

Activity of water = 1.000

Ionic strength = 5.137e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.465e-003

Total CO2 (mol/kg) = 3.465e-003

Temperature (deg C) = 25.020

Electrical balance (eq) = -1.199e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.76

Iterations = 6

Total H = 1.110157e+002

Total O = 5.551690e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8438 0.7598

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.426e-007 3.170e-007 -6.465 -6.499 -0.034

H+ 3.389e-008 3.162e-008 -7.470 -7.500 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.465e-003

HCO3- 3.193e-003 2.963e-003 -2.496 -2.528 -0.032

CO2 2.104e-004 2.107e-004 -3.677 -3.676 0.001

CaHCO3+ 3.447e-005 3.199e-005 -4.463 -4.495 -0.032

MgHCO3+ 1.384e-005 1.282e-005 -4.859 -4.892 -0.033

CaCO3 6.243e-006 6.250e-006 -5.205 -5.204 0.001

CO3-2 5.925e-006 4.396e-006 -5.227 -5.357 -0.130

MgCO3 1.550e-006 1.552e-006 -5.810 -5.809 0.001

NaHCO3 1.541e-008 1.543e-008 -7.812 -7.812 0.001

NaCO3- 8.190e-010 7.586e-010 -9.087 -9.120 -0.033

Ca 1.193e-003

Ca+2 1.141e-003 8.459e-004 -2.943 -3.073 -0.130

CaHCO3+ 3.447e-005 3.199e-005 -4.463 -4.495 -0.032

CaSO4 1.211e-005 1.212e-005 -4.917 -4.916 0.001

CaCO3 6.243e-006 6.250e-006 -5.205 -5.204 0.001

CaOH+ 4.793e-009 4.439e-009 -8.319 -8.353 -0.033

CaHSO4+ 2.425e-012 2.246e-012 -11.615 -11.649 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.300e-005 -4.242 -4.276 -0.034

H(0) 1.414e-026

H2 7.070e-027 7.078e-027 -26.151 -26.150 0.001

K 3.326e-006

K+ 3.324e-006 3.076e-006 -5.478 -5.512 -0.034

KSO4- 1.676e-009 1.552e-009 -8.776 -8.809 -0.033

KOH 3.369e-013 3.373e-013 -12.473 -12.472 0.001

Mg 5.184e-004

Mg+2 4.967e-004 3.697e-004 -3.304 -3.432 -0.128

MgHCO3+ 1.384e-005 1.282e-005 -4.859 -4.892 -0.033

MgSO4 6.219e-006 6.226e-006 -5.206 -5.206 0.001

MgCO3 1.550e-006 1.552e-006 -5.810 -5.809 0.001

MgOH+ 4.591e-008 4.252e-008 -7.338 -7.371 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.257e-006 -5.001 -5.034 -0.033

NaHCO3 1.541e-008 1.543e-008 -7.812 -7.812 0.001

NaSO4- 3.597e-009 3.331e-009 -8.444 -8.477 -0.033

NaCO3- 8.190e-010 7.586e-010 -9.087 -9.120 -0.033

NaOH 1.932e-012 1.934e-012 -11.714 -11.714 0.001

O(0) 4.001e-005

O2 2.001e-005 2.003e-005 -4.699 -4.698 0.001

S(6) 1.154e-004

SO4-2 9.704e-005 7.180e-005 -4.013 -4.144 -0.131

CaSO4 1.211e-005 1.212e-005 -4.917 -4.916 0.001

MgSO4 6.219e-006 6.226e-006 -5.206 -5.206 0.001

NaSO4- 3.597e-009 3.331e-009 -8.444 -8.477 -0.033

KSO4- 1.676e-009 1.552e-009 -8.776 -8.809 -0.033

HSO4- 2.384e-010 2.208e-010 -9.623 -9.656 -0.033

CaHSO4+ 2.425e-012 2.246e-012 -11.615 -11.649 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.86 -7.22 -4.36 CaSO4

Aragonite -0.09 -8.43 -8.34 CaCO3

Calcite 0.05 -8.43 -8.48 CaCO3

CO2(g) -2.21 -3.68 -1.47 CO2

Dolomite -0.13 -17.22 -17.09 CaMg(CO3)2

Gypsum -2.64 -7.22 -4.58 CaSO4:2H2O

H2(g) -23.00 -26.15 -3.15 H2

H2O(g) -1.51 -0.00 1.51 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -1.81 -4.70 -2.89 O2

Initial solution 69. 30/8/2012 04:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.279e-003 3.279e-003

Ca 1.197e-003 1.197e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 2.626e-005 2.626e-005

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.480

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 323

Density (g/cm3) = 0.99728

Activity of water = 1.000

Ionic strength = 5.150e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.487e-003

Total CO2 (mol/kg) = 3.487e-003

Temperature (deg C) = 24.960

Electrical balance (eq) = -1.229e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.80

Iterations = 6

Total H = 1.110157e+002

Total O = 5.551695e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8230 0.7585

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.257e-007 3.014e-007 -6.487 -6.521 -0.034

H+ 3.549e-008 3.311e-008 -7.450 -7.480 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.487e-003

HCO3- 3.204e-003 2.974e-003 -2.494 -2.527 -0.032

CO2 2.213e-004 2.215e-004 -3.655 -3.655 0.001

CaHCO3+ 3.467e-005 3.217e-005 -4.460 -4.493 -0.032

MgHCO3+ 1.388e-005 1.286e-005 -4.857 -4.891 -0.033

CaCO3 5.986e-006 5.993e-006 -5.223 -5.222 0.001

CO3-2 5.673e-006 4.208e-006 -5.246 -5.376 -0.130

MgCO3 1.482e-006 1.483e-006 -5.829 -5.829 0.001

NaHCO3 1.546e-008 1.548e-008 -7.811 -7.810 0.001

NaCO3- 7.816e-010 7.239e-010 -9.107 -9.140 -0.033

Ca 1.197e-003

Ca+2 1.144e-003 8.485e-004 -2.941 -3.071 -0.130

CaHCO3+ 3.467e-005 3.217e-005 -4.460 -4.493 -0.032

CaSO4 1.213e-005 1.215e-005 -4.916 -4.916 0.001

CaCO3 5.986e-006 5.993e-006 -5.223 -5.222 0.001

CaOH+ 4.591e-009 4.252e-009 -8.338 -8.371 -0.033

CaHSO4+ 2.543e-012 2.355e-012 -11.595 -11.628 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.300e-005 -4.242 -4.276 -0.034

H(0) 1.551e-026

H2 7.756e-027 7.766e-027 -26.110 -26.110 0.001

K 3.326e-006

K+ 3.324e-006 3.076e-006 -5.478 -5.512 -0.034

KSO4- 1.674e-009 1.550e-009 -8.776 -8.810 -0.033

KOH 3.217e-013 3.220e-013 -12.493 -12.492 0.001

Mg 5.184e-004

Mg+2 4.968e-004 3.696e-004 -3.304 -3.432 -0.128

MgHCO3+ 1.388e-005 1.286e-005 -4.857 -4.891 -0.033

MgSO4 6.205e-006 6.212e-006 -5.207 -5.207 0.001

MgCO3 1.482e-006 1.483e-006 -5.829 -5.829 0.001

MgOH+ 4.360e-008 4.038e-008 -7.361 -7.394 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.256e-006 -5.001 -5.034 -0.033

NaHCO3 1.546e-008 1.548e-008 -7.811 -7.810 0.001

NaSO4- 3.594e-009 3.329e-009 -8.444 -8.478 -0.033

NaCO3- 7.816e-010 7.239e-010 -9.107 -9.140 -0.033

NaOH 1.845e-012 1.847e-012 -11.734 -11.734 0.001

O(0) 2.626e-005

O2 1.313e-005 1.314e-005 -4.882 -4.881 0.001

S(6) 1.154e-004

SO4-2 9.703e-005 7.177e-005 -4.013 -4.144 -0.131

CaSO4 1.213e-005 1.215e-005 -4.916 -4.916 0.001

MgSO4 6.205e-006 6.212e-006 -5.207 -5.207 0.001

NaSO4- 3.594e-009 3.329e-009 -8.444 -8.478 -0.033

KSO4- 1.674e-009 1.550e-009 -8.776 -8.810 -0.033

HSO4- 2.492e-010 2.308e-010 -9.603 -9.637 -0.033

CaHSO4+ 2.543e-012 2.355e-012 -11.595 -11.628 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.22 -4.36 CaSO4

Aragonite -0.11 -8.45 -8.34 CaCO3

Calcite 0.03 -8.45 -8.48 CaCO3

CO2(g) -2.19 -3.65 -1.47 CO2

Dolomite -0.17 -17.26 -17.09 CaMg(CO3)2

Gypsum -2.63 -7.22 -4.58 CaSO4:2H2O

H2(g) -22.96 -26.11 -3.15 H2

H2O(g) -1.51 -0.00 1.51 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -1.99 -4.88 -2.89 O2

Initial solution 70. 30/8/2012 05:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.279e-003 3.279e-003

Ca 1.197e-003 1.197e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.938e-005 1.938e-005

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.470

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 322

Density (g/cm3) = 0.99730

Activity of water = 1.000

Ionic strength = 5.150e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.493e-003

Total CO2 (mol/kg) = 3.493e-003

Temperature (deg C) = 24.880

Electrical balance (eq) = -1.229e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.80

Iterations = 6

Total H = 1.110157e+002

Total O = 5.551695e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8067 0.7573

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.164e-007 2.927e-007 -6.500 -6.534 -0.034

H+ 3.632e-008 3.388e-008 -7.440 -7.470 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.493e-003

HCO3- 3.205e-003 2.974e-003 -2.494 -2.527 -0.032

CO2 2.267e-004 2.270e-004 -3.645 -3.644 0.001

CaHCO3+ 3.464e-005 3.215e-005 -4.460 -4.493 -0.032

MgHCO3+ 1.388e-005 1.286e-005 -4.857 -4.891 -0.033

CaCO3 5.834e-006 5.841e-006 -5.234 -5.234 0.001

CO3-2 5.536e-006 4.107e-006 -5.257 -5.387 -0.130

MgCO3 1.444e-006 1.446e-006 -5.840 -5.840 0.001

NaHCO3 1.546e-008 1.548e-008 -7.811 -7.810 0.001

NaCO3- 7.596e-010 7.036e-010 -9.119 -9.153 -0.033

Ca 1.197e-003

Ca+2 1.145e-003 8.487e-004 -2.941 -3.071 -0.130

CaHCO3+ 3.464e-005 3.215e-005 -4.460 -4.493 -0.032

CaSO4 1.213e-005 1.214e-005 -4.916 -4.916 0.001

CaCO3 5.834e-006 5.841e-006 -5.234 -5.234 0.001

CaOH+ 4.487e-009 4.156e-009 -8.348 -8.381 -0.033

CaHSO4+ 2.598e-012 2.406e-012 -11.585 -11.619 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.300e-005 -4.242 -4.276 -0.034

H(0) 1.626e-026

H2 8.128e-027 8.138e-027 -26.090 -26.089 0.001

K 3.326e-006

K+ 3.324e-006 3.076e-006 -5.478 -5.512 -0.034

KSO4- 1.671e-009 1.548e-009 -8.777 -8.810 -0.033

KOH 3.143e-013 3.147e-013 -12.503 -12.502 0.001

Mg 5.184e-004

Mg+2 4.968e-004 3.697e-004 -3.304 -3.432 -0.128

MgHCO3+ 1.388e-005 1.286e-005 -4.857 -4.891 -0.033

MgSO4 6.194e-006 6.202e-006 -5.208 -5.207 0.001

MgCO3 1.444e-006 1.446e-006 -5.840 -5.840 0.001

MgOH+ 4.231e-008 3.918e-008 -7.374 -7.407 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.256e-006 -5.001 -5.034 -0.033

NaHCO3 1.546e-008 1.548e-008 -7.811 -7.810 0.001

NaSO4- 3.593e-009 3.327e-009 -8.445 -8.478 -0.033

NaCO3- 7.596e-010 7.036e-010 -9.119 -9.153 -0.033

NaOH 1.803e-012 1.805e-012 -11.744 -11.744 0.001

O(0) 1.938e-005

O2 9.690e-006 9.702e-006 -5.014 -5.013 0.001

S(6) 1.154e-004

SO4-2 9.705e-005 7.178e-005 -4.013 -4.144 -0.131

CaSO4 1.213e-005 1.214e-005 -4.916 -4.916 0.001

MgSO4 6.194e-006 6.202e-006 -5.208 -5.207 0.001

NaSO4- 3.593e-009 3.327e-009 -8.445 -8.478 -0.033

KSO4- 1.671e-009 1.548e-009 -8.777 -8.810 -0.033

HSO4- 2.547e-010 2.359e-010 -9.594 -9.627 -0.033

CaHSO4+ 2.598e-012 2.406e-012 -11.585 -11.619 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.22 -4.36 CaSO4

Aragonite -0.12 -8.46 -8.34 CaCO3

Calcite 0.02 -8.46 -8.48 CaCO3

CO2(g) -2.18 -3.64 -1.47 CO2

Dolomite -0.19 -17.28 -17.09 CaMg(CO3)2

Gypsum -2.63 -7.22 -4.58 CaSO4:2H2O

H2(g) -22.94 -26.09 -3.15 H2

H2O(g) -1.51 -0.00 1.51 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -2.12 -5.01 -2.89 O2

Initial solution 71. 30/8/2012 05:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.290e-003 3.290e-003

Ca 1.201e-003 1.201e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.125e-005 1.125e-005

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.470

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 322

Density (g/cm3) = 0.99732

Activity of water = 1.000

Ionic strength = 5.162e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.504e-003

Total CO2 (mol/kg) = 3.504e-003

Temperature (deg C) = 24.820

Electrical balance (eq) = -1.256e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.84

Iterations = 6

Total H = 1.110157e+002

Total O = 5.551697e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.7526 0.7539

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.150e-007 2.914e-007 -6.502 -6.535 -0.034

H+ 3.632e-008 3.388e-008 -7.440 -7.470 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.504e-003

HCO3- 3.215e-003 2.983e-003 -2.493 -2.525 -0.032

CO2 2.275e-004 2.278e-004 -3.643 -3.642 0.001

CaHCO3+ 3.481e-005 3.230e-005 -4.458 -4.491 -0.032

MgHCO3+ 1.392e-005 1.289e-005 -4.856 -4.890 -0.033

CaCO3 5.854e-006 5.860e-006 -5.233 -5.232 0.001

CO3-2 5.547e-006 4.114e-006 -5.256 -5.386 -0.130

MgCO3 1.445e-006 1.447e-006 -5.840 -5.840 0.001

NaHCO3 1.551e-008 1.553e-008 -7.809 -7.809 0.001

NaCO3- 7.587e-010 7.026e-010 -9.120 -9.153 -0.033

Ca 1.201e-003

Ca+2 1.148e-003 8.510e-004 -2.940 -3.070 -0.130

CaHCO3+ 3.481e-005 3.230e-005 -4.458 -4.491 -0.032

CaSO4 1.215e-005 1.216e-005 -4.915 -4.915 0.001

CaCO3 5.854e-006 5.860e-006 -5.233 -5.232 0.001

CaOH+ 4.500e-009 4.168e-009 -8.347 -8.380 -0.033

CaHSO4+ 2.601e-012 2.409e-012 -11.585 -11.618 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.300e-005 -4.242 -4.276 -0.034

H(0) 1.627e-026

H2 8.133e-027 8.143e-027 -26.090 -26.089 0.001

K 3.326e-006

K+ 3.324e-006 3.076e-006 -5.478 -5.512 -0.034

KSO4- 1.669e-009 1.546e-009 -8.778 -8.811 -0.033

KOH 3.143e-013 3.147e-013 -12.503 -12.502 0.001

Mg 5.184e-004

Mg+2 4.968e-004 3.696e-004 -3.304 -3.432 -0.128

MgHCO3+ 1.392e-005 1.289e-005 -4.856 -4.890 -0.033

MgSO4 6.180e-006 6.188e-006 -5.209 -5.208 0.001

MgCO3 1.445e-006 1.447e-006 -5.840 -5.840 0.001

MgOH+ 4.207e-008 3.896e-008 -7.376 -7.409 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.256e-006 -5.001 -5.034 -0.033

NaHCO3 1.551e-008 1.553e-008 -7.809 -7.809 0.001

NaSO4- 3.590e-009 3.325e-009 -8.445 -8.478 -0.033

NaCO3- 7.587e-010 7.026e-010 -9.120 -9.153 -0.033

NaOH 1.802e-012 1.805e-012 -11.744 -11.744 0.001

O(0) 1.125e-005

O2 5.627e-006 5.633e-006 -5.250 -5.249 0.001

S(6) 1.154e-004

SO4-2 9.704e-005 7.175e-005 -4.013 -4.144 -0.131

CaSO4 1.215e-005 1.216e-005 -4.915 -4.915 0.001

MgSO4 6.180e-006 6.188e-006 -5.209 -5.208 0.001

NaSO4- 3.590e-009 3.325e-009 -8.445 -8.478 -0.033

KSO4- 1.669e-009 1.546e-009 -8.778 -8.811 -0.033

HSO4- 2.542e-010 2.355e-010 -9.595 -9.628 -0.033

CaHSO4+ 2.601e-012 2.409e-012 -11.585 -11.618 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite -0.12 -8.46 -8.33 CaCO3

Calcite 0.02 -8.46 -8.48 CaCO3

CO2(g) -2.18 -3.64 -1.47 CO2

Dolomite -0.19 -17.27 -17.09 CaMg(CO3)2

Gypsum -2.63 -7.21 -4.58 CaSO4:2H2O

H2(g) -22.94 -26.09 -3.15 H2

H2O(g) -1.51 -0.00 1.51 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -2.36 -5.25 -2.89 O2

Initial solution 72. 30/8/2012 05:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.300e-003 3.300e-003

Ca 1.205e-003 1.205e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 8.127e-006 8.127e-006

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.480

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 323

Density (g/cm3) = 0.99734

Activity of water = 1.000

Ionic strength = 5.174e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.510e-003

Total CO2 (mol/kg) = 3.510e-003

Temperature (deg C) = 24.750

Electrical balance (eq) = -1.284e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.88

Iterations = 6

Total H = 1.110157e+002

Total O = 5.551699e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.7131 0.7514

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.206e-007 2.966e-007 -6.494 -6.528 -0.034

H+ 3.550e-008 3.311e-008 -7.450 -7.480 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.510e-003

HCO3- 3.224e-003 2.992e-003 -2.492 -2.524 -0.032

CO2 2.232e-004 2.235e-004 -3.651 -3.651 0.001

CaHCO3+ 3.497e-005 3.245e-005 -4.456 -4.489 -0.032

MgHCO3+ 1.395e-005 1.292e-005 -4.855 -4.889 -0.033

CaCO3 6.006e-006 6.014e-006 -5.221 -5.221 0.001

CO3-2 5.686e-006 4.216e-006 -5.245 -5.375 -0.130

MgCO3 1.479e-006 1.481e-006 -5.830 -5.830 0.001

NaHCO3 1.555e-008 1.557e-008 -7.808 -7.808 0.001

NaCO3- 7.748e-010 7.175e-010 -9.111 -9.144 -0.033

Ca 1.205e-003

Ca+2 1.152e-003 8.533e-004 -2.939 -3.069 -0.130

CaHCO3+ 3.497e-005 3.245e-005 -4.456 -4.489 -0.032

CaSO4 1.217e-005 1.218e-005 -4.915 -4.914 0.001

CaCO3 6.006e-006 6.014e-006 -5.221 -5.221 0.001

CaOH+ 4.618e-009 4.276e-009 -8.336 -8.369 -0.033

CaHSO4+ 2.544e-012 2.356e-012 -11.594 -11.628 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.299e-005 -4.242 -4.276 -0.034

H(0) 1.555e-026

H2 7.773e-027 7.782e-027 -26.109 -26.109 0.001

K 3.326e-006

K+ 3.324e-006 3.075e-006 -5.478 -5.512 -0.034

KSO4- 1.667e-009 1.543e-009 -8.778 -8.812 -0.033

KOH 3.216e-013 3.220e-013 -12.493 -12.492 0.001

Mg 5.184e-004

Mg+2 4.968e-004 3.694e-004 -3.304 -3.432 -0.129

MgHCO3+ 1.395e-005 1.292e-005 -4.855 -4.889 -0.033

MgSO4 6.165e-006 6.172e-006 -5.210 -5.210 0.001

MgCO3 1.479e-006 1.481e-006 -5.830 -5.830 0.001

MgOH+ 4.276e-008 3.960e-008 -7.369 -7.402 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.255e-006 -5.001 -5.034 -0.033

NaHCO3 1.555e-008 1.557e-008 -7.808 -7.808 0.001

NaSO4- 3.587e-009 3.322e-009 -8.445 -8.479 -0.033

NaCO3- 7.748e-010 7.175e-010 -9.111 -9.144 -0.033

NaOH 1.844e-012 1.846e-012 -11.734 -11.734 0.001

O(0) 8.127e-006

O2 4.064e-006 4.068e-006 -5.391 -5.391 0.001

S(6) 1.154e-004

SO4-2 9.703e-005 7.173e-005 -4.013 -4.144 -0.131

CaSO4 1.217e-005 1.218e-005 -4.915 -4.914 0.001

MgSO4 6.165e-006 6.172e-006 -5.210 -5.210 0.001

NaSO4- 3.587e-009 3.322e-009 -8.445 -8.479 -0.033

KSO4- 1.667e-009 1.543e-009 -8.778 -8.812 -0.033

HSO4- 2.480e-010 2.297e-010 -9.606 -9.639 -0.033

CaHSO4+ 2.544e-012 2.356e-012 -11.594 -11.628 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite -0.11 -8.44 -8.33 CaCO3

Calcite 0.03 -8.44 -8.48 CaCO3

CO2(g) -2.19 -3.65 -1.46 CO2

Dolomite -0.17 -17.25 -17.08 CaMg(CO3)2

Gypsum -2.63 -7.21 -4.58 CaSO4:2H2O

H2(g) -22.96 -26.11 -3.15 H2

H2O(g) -1.52 -0.00 1.52 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -2.50 -5.39 -2.89 O2

Initial solution 73. 30/8/2012 05:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.300e-003 3.300e-003

Ca 1.205e-003 1.205e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.627e-006 5.627e-006

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.480

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 322

Density (g/cm3) = 0.99735

Activity of water = 1.000

Ionic strength = 5.174e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.510e-003

Total CO2 (mol/kg) = 3.510e-003

Temperature (deg C) = 24.700

Electrical balance (eq) = -1.284e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.88

Iterations = 6

Total H = 1.110157e+002

Total O = 5.551699e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.6773 0.7492

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.194e-007 2.955e-007 -6.496 -6.529 -0.034

H+ 3.550e-008 3.311e-008 -7.450 -7.480 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.510e-003

HCO3- 3.224e-003 2.992e-003 -2.492 -2.524 -0.032

CO2 2.233e-004 2.236e-004 -3.651 -3.651 0.001

CaHCO3+ 3.494e-005 3.243e-005 -4.457 -4.489 -0.032

MgHCO3+ 1.395e-005 1.292e-005 -4.855 -4.889 -0.033

CaCO3 5.995e-006 6.002e-006 -5.222 -5.222 0.001

CO3-2 5.680e-006 4.212e-006 -5.246 -5.376 -0.130

MgCO3 1.476e-006 1.478e-006 -5.831 -5.830 0.001

NaHCO3 1.555e-008 1.557e-008 -7.808 -7.808 0.001

NaCO3- 7.720e-010 7.149e-010 -9.112 -9.146 -0.033

Ca 1.205e-003

Ca+2 1.152e-003 8.534e-004 -2.939 -3.069 -0.130

CaHCO3+ 3.494e-005 3.243e-005 -4.457 -4.489 -0.032

CaSO4 1.217e-005 1.218e-005 -4.915 -4.914 0.001

CaCO3 5.995e-006 6.002e-006 -5.222 -5.222 0.001

CaOH+ 4.618e-009 4.277e-009 -8.336 -8.369 -0.033

CaHSO4+ 2.542e-012 2.354e-012 -11.595 -11.628 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.299e-005 -4.242 -4.276 -0.034

H(0) 1.555e-026

H2 7.776e-027 7.786e-027 -26.109 -26.109 0.001

K 3.326e-006

K+ 3.324e-006 3.075e-006 -5.478 -5.512 -0.034

KSO4- 1.665e-009 1.542e-009 -8.779 -8.812 -0.033

KOH 3.216e-013 3.220e-013 -12.493 -12.492 0.001

Mg 5.184e-004

Mg+2 4.968e-004 3.695e-004 -3.304 -3.432 -0.129

MgHCO3+ 1.395e-005 1.292e-005 -4.855 -4.889 -0.033

MgSO4 6.158e-006 6.165e-006 -5.211 -5.210 0.001

MgCO3 1.476e-006 1.478e-006 -5.831 -5.830 0.001

MgOH+ 4.257e-008 3.942e-008 -7.371 -7.404 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.255e-006 -5.001 -5.034 -0.033

NaHCO3 1.555e-008 1.557e-008 -7.808 -7.808 0.001

NaSO4- 3.587e-009 3.321e-009 -8.445 -8.479 -0.033

NaCO3- 7.720e-010 7.149e-010 -9.112 -9.146 -0.033

NaOH 1.844e-012 1.846e-012 -11.734 -11.734 0.001

O(0) 5.627e-006

O2 2.813e-006 2.817e-006 -5.551 -5.550 0.001

S(6) 1.154e-004

SO4-2 9.704e-005 7.174e-005 -4.013 -4.144 -0.131

CaSO4 1.217e-005 1.218e-005 -4.915 -4.914 0.001

MgSO4 6.158e-006 6.165e-006 -5.211 -5.210 0.001

NaSO4- 3.587e-009 3.321e-009 -8.445 -8.479 -0.033

KSO4- 1.665e-009 1.542e-009 -8.779 -8.812 -0.033

HSO4- 2.478e-010 2.294e-010 -9.606 -9.639 -0.033

CaHSO4+ 2.542e-012 2.354e-012 -11.595 -11.628 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite -0.11 -8.44 -8.33 CaCO3

Calcite 0.03 -8.44 -8.48 CaCO3

CO2(g) -2.19 -3.65 -1.46 CO2

Dolomite -0.17 -17.25 -17.08 CaMg(CO3)2

Gypsum -2.63 -7.21 -4.58 CaSO4:2H2O

H2(g) -22.96 -26.11 -3.15 H2

H2O(g) -1.52 -0.00 1.52 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -2.66 -5.55 -2.89 O2

Initial solution 74. 30/8/2012 06:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.310e-003 3.310e-003

Ca 1.208e-003 1.208e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.376e-006 4.376e-006

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.480

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 322

Density (g/cm3) = 0.99737

Activity of water = 1.000

Ionic strength = 5.187e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.521e-003

Total CO2 (mol/kg) = 3.521e-003

Temperature (deg C) = 24.620

Electrical balance (eq) = -1.314e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.91

Iterations = 6

Total H = 1.110157e+002

Total O = 5.551702e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.6567 0.7478

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.175e-007 2.937e-007 -6.498 -6.532 -0.034

H+ 3.550e-008 3.311e-008 -7.450 -7.480 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.521e-003

HCO3- 3.235e-003 3.001e-003 -2.490 -2.523 -0.033

CO2 2.243e-004 2.245e-004 -3.649 -3.649 0.001

CaHCO3+ 3.511e-005 3.258e-005 -4.455 -4.487 -0.033

MgHCO3+ 1.398e-005 1.295e-005 -4.854 -4.888 -0.033

CaCO3 6.011e-006 6.018e-006 -5.221 -5.221 0.001

CO3-2 5.690e-006 4.218e-006 -5.245 -5.375 -0.130

MgCO3 1.476e-006 1.478e-006 -5.831 -5.830 0.001

NaHCO3 1.560e-008 1.562e-008 -7.807 -7.806 0.001

NaCO3- 7.701e-010 7.131e-010 -9.113 -9.147 -0.033

Ca 1.208e-003

Ca+2 1.155e-003 8.558e-004 -2.937 -3.068 -0.130

CaHCO3+ 3.511e-005 3.258e-005 -4.455 -4.487 -0.033

CaSO4 1.219e-005 1.220e-005 -4.914 -4.914 0.001

CaCO3 6.011e-006 6.018e-006 -5.221 -5.221 0.001

CaOH+ 4.631e-009 4.289e-009 -8.334 -8.368 -0.033

CaHSO4+ 2.544e-012 2.356e-012 -11.594 -11.628 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.299e-005 -4.242 -4.276 -0.034

H(0) 1.557e-026

H2 7.783e-027 7.792e-027 -26.109 -26.108 0.001

K 3.326e-006

K+ 3.324e-006 3.075e-006 -5.478 -5.512 -0.034

KSO4- 1.662e-009 1.539e-009 -8.779 -8.813 -0.033

KOH 3.216e-013 3.220e-013 -12.493 -12.492 0.001

Mg 5.184e-004

Mg+2 4.968e-004 3.693e-004 -3.304 -3.433 -0.129

MgHCO3+ 1.398e-005 1.295e-005 -4.854 -4.888 -0.033

MgSO4 6.141e-006 6.149e-006 -5.212 -5.211 0.001

MgCO3 1.476e-006 1.478e-006 -5.831 -5.830 0.001

MgOH+ 4.225e-008 3.913e-008 -7.374 -7.408 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.254e-006 -5.001 -5.034 -0.033

NaHCO3 1.560e-008 1.562e-008 -7.807 -7.806 0.001

NaSO4- 3.584e-009 3.318e-009 -8.446 -8.479 -0.033

NaCO3- 7.701e-010 7.131e-010 -9.113 -9.147 -0.033

NaOH 1.844e-012 1.846e-012 -11.734 -11.734 0.001

O(0) 4.376e-006

O2 2.188e-006 2.191e-006 -5.660 -5.659 0.001

S(6) 1.154e-004

SO4-2 9.704e-005 7.172e-005 -4.013 -4.144 -0.131

CaSO4 1.219e-005 1.220e-005 -4.914 -4.914 0.001

MgSO4 6.141e-006 6.149e-006 -5.212 -5.211 0.001

NaSO4- 3.584e-009 3.318e-009 -8.446 -8.479 -0.033

KSO4- 1.662e-009 1.539e-009 -8.779 -8.813 -0.033

HSO4- 2.473e-010 2.290e-010 -9.607 -9.640 -0.033

CaHSO4+ 2.544e-012 2.356e-012 -11.594 -11.628 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite -0.11 -8.44 -8.33 CaCO3

Calcite 0.04 -8.44 -8.48 CaCO3

CO2(g) -2.19 -3.65 -1.46 CO2

Dolomite -0.17 -17.25 -17.08 CaMg(CO3)2

Gypsum -2.63 -7.21 -4.58 CaSO4:2H2O

H2(g) -22.96 -26.11 -3.15 H2

H2O(g) -1.52 -0.00 1.52 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -2.77 -5.66 -2.89 O2

Initial solution 75. 30/8/2012 06:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.321e-003 3.321e-003

Ca 1.212e-003 1.212e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.126e-006 3.126e-006

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.490

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 323

Density (g/cm3) = 0.99738

Activity of water = 1.000

Ionic strength = 5.198e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.527e-003

Total CO2 (mol/kg) = 3.527e-003

Temperature (deg C) = 24.570

Electrical balance (eq) = -1.342e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.95

Iterations = 6

Total H = 1.110157e+002

Total O = 5.551704e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.6143 0.7451

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.237e-007 2.994e-007 -6.490 -6.524 -0.034

H+ 3.469e-008 3.236e-008 -7.460 -7.490 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.527e-003

HCO3- 3.244e-003 3.010e-003 -2.489 -2.521 -0.033

CO2 2.199e-004 2.202e-004 -3.658 -3.657 0.001

CaHCO3+ 3.528e-005 3.273e-005 -4.452 -4.485 -0.033

MgHCO3+ 1.402e-005 1.298e-005 -4.853 -4.887 -0.033

CaCO3 6.172e-006 6.180e-006 -5.210 -5.209 0.001

CO3-2 5.835e-006 4.324e-006 -5.234 -5.364 -0.130

MgCO3 1.512e-006 1.513e-006 -5.821 -5.820 0.001

NaHCO3 1.564e-008 1.566e-008 -7.806 -7.805 0.001

NaCO3- 7.874e-010 7.291e-010 -9.104 -9.137 -0.033

Ca 1.212e-003

Ca+2 1.158e-003 8.580e-004 -2.936 -3.066 -0.130

CaHCO3+ 3.528e-005 3.273e-005 -4.452 -4.485 -0.033

CaSO4 1.221e-005 1.222e-005 -4.913 -4.913 0.001

CaCO3 6.172e-006 6.180e-006 -5.210 -5.209 0.001

CaOH+ 4.752e-009 4.400e-009 -8.323 -8.357 -0.033

CaHSO4+ 2.489e-012 2.305e-012 -11.604 -11.637 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.299e-005 -4.242 -4.276 -0.034

H(0) 1.487e-026

H2 7.436e-027 7.445e-027 -26.129 -26.128 0.001

K 3.326e-006

K+ 3.324e-006 3.075e-006 -5.478 -5.512 -0.034

KSO4- 1.660e-009 1.537e-009 -8.780 -8.813 -0.033

KOH 3.291e-013 3.295e-013 -12.483 -12.482 0.001

Mg 5.184e-004

Mg+2 4.967e-004 3.692e-004 -3.304 -3.433 -0.129

MgHCO3+ 1.402e-005 1.298e-005 -4.853 -4.887 -0.033

MgSO4 6.129e-006 6.136e-006 -5.213 -5.212 0.001

MgCO3 1.512e-006 1.513e-006 -5.821 -5.820 0.001

MgOH+ 4.303e-008 3.984e-008 -7.366 -7.400 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.254e-006 -5.001 -5.034 -0.033

NaHCO3 1.564e-008 1.566e-008 -7.806 -7.805 0.001

NaSO4- 3.581e-009 3.316e-009 -8.446 -8.479 -0.033

NaCO3- 7.874e-010 7.291e-010 -9.104 -9.137 -0.033

NaOH 1.887e-012 1.889e-012 -11.724 -11.724 0.001

O(0) 3.126e-006

O2 1.563e-006 1.565e-006 -5.806 -5.806 0.001

S(6) 1.154e-004

SO4-2 9.703e-005 7.169e-005 -4.013 -4.145 -0.131

CaSO4 1.221e-005 1.222e-005 -4.913 -4.913 0.001

MgSO4 6.129e-006 6.136e-006 -5.213 -5.212 0.001

NaSO4- 3.581e-009 3.316e-009 -8.446 -8.479 -0.033

KSO4- 1.660e-009 1.537e-009 -8.780 -8.813 -0.033

HSO4- 2.413e-010 2.234e-010 -9.617 -9.651 -0.033

CaHSO4+ 2.489e-012 2.305e-012 -11.604 -11.637 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite -0.10 -8.43 -8.33 CaCO3

Calcite 0.05 -8.43 -8.48 CaCO3

CO2(g) -2.19 -3.66 -1.46 CO2

Dolomite -0.15 -17.23 -17.08 CaMg(CO3)2

Gypsum -2.63 -7.21 -4.58 CaSO4:2H2O

H2(g) -22.98 -26.13 -3.15 H2

H2O(g) -1.52 -0.00 1.52 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -2.92 -5.81 -2.89 O2

Initial solution 76. 30/8/2012 06:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.341e-003 3.341e-003

Ca 1.220e-003 1.220e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.126e-006 3.126e-006

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.480

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 324

Density (g/cm3) = 0.99740

Activity of water = 1.000

Ionic strength = 5.223e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.554e-003

Total CO2 (mol/kg) = 3.554e-003

Temperature (deg C) = 24.500

Electrical balance (eq) = -1.399e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.02

Iterations = 6

Total H = 1.110157e+002

Total O = 5.551712e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.6301 0.7459

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.147e-007 2.910e-007 -6.502 -6.536 -0.034

H+ 3.551e-008 3.311e-008 -7.450 -7.480 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.554e-003

HCO3- 3.265e-003 3.029e-003 -2.486 -2.519 -0.033

CO2 2.266e-004 2.269e-004 -3.645 -3.644 0.001

CaHCO3+ 3.566e-005 3.308e-005 -4.448 -4.480 -0.033

MgHCO3+ 1.409e-005 1.305e-005 -4.851 -4.885 -0.033

CaCO3 6.086e-006 6.093e-006 -5.216 -5.215 0.001

CO3-2 5.733e-006 4.246e-006 -5.242 -5.372 -0.130

MgCO3 1.482e-006 1.484e-006 -5.829 -5.829 0.001

NaHCO3 1.574e-008 1.576e-008 -7.803 -7.803 0.001

NaCO3- 7.705e-010 7.133e-010 -9.113 -9.147 -0.033

Ca 1.220e-003

Ca+2 1.166e-003 8.628e-004 -2.933 -3.064 -0.131

CaHCO3+ 3.566e-005 3.308e-005 -4.448 -4.480 -0.033

CaSO4 1.226e-005 1.227e-005 -4.912 -4.911 0.001

CaCO3 6.086e-006 6.093e-006 -5.216 -5.215 0.001

CaOH+ 4.671e-009 4.324e-009 -8.331 -8.364 -0.033

CaHSO4+ 2.556e-012 2.366e-012 -11.592 -11.626 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.298e-005 -4.242 -4.276 -0.034

H(0) 1.558e-026

H2 7.792e-027 7.801e-027 -26.108 -26.108 0.001

K 3.326e-006

K+ 3.324e-006 3.074e-006 -5.478 -5.512 -0.034

KSO4- 1.657e-009 1.534e-009 -8.781 -8.814 -0.033

KOH 3.215e-013 3.219e-013 -12.493 -12.492 0.001

Mg 5.184e-004

Mg+2 4.967e-004 3.690e-004 -3.304 -3.433 -0.129

MgHCO3+ 1.409e-005 1.305e-005 -4.851 -4.885 -0.033

MgSO4 6.108e-006 6.116e-006 -5.214 -5.214 0.001

MgCO3 1.482e-006 1.484e-006 -5.829 -5.829 0.001

MgOH+ 4.177e-008 3.866e-008 -7.379 -7.413 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.252e-006 -5.001 -5.034 -0.033

NaHCO3 1.574e-008 1.576e-008 -7.803 -7.803 0.001

NaSO4- 3.576e-009 3.311e-009 -8.447 -8.480 -0.033

NaCO3- 7.705e-010 7.133e-010 -9.113 -9.147 -0.033

NaOH 1.844e-012 1.846e-012 -11.734 -11.734 0.001

O(0) 3.126e-006

O2 1.563e-006 1.565e-006 -5.806 -5.806 0.001

S(6) 1.154e-004

SO4-2 9.700e-005 7.162e-005 -4.013 -4.145 -0.132

CaSO4 1.226e-005 1.227e-005 -4.912 -4.911 0.001

MgSO4 6.108e-006 6.116e-006 -5.214 -5.214 0.001

NaSO4- 3.576e-009 3.311e-009 -8.447 -8.480 -0.033

KSO4- 1.657e-009 1.534e-009 -8.781 -8.814 -0.033

HSO4- 2.464e-010 2.281e-010 -9.608 -9.642 -0.033

CaHSO4+ 2.556e-012 2.366e-012 -11.592 -11.626 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite -0.10 -8.44 -8.33 CaCO3

Calcite 0.04 -8.44 -8.48 CaCO3

CO2(g) -2.18 -3.64 -1.46 CO2

Dolomite -0.16 -17.24 -17.08 CaMg(CO3)2

Gypsum -2.63 -7.21 -4.58 CaSO4:2H2O

H2(g) -22.96 -26.11 -3.15 H2

H2O(g) -1.52 -0.00 1.52 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -2.92 -5.81 -2.89 O2

Initial solution 77. 30/8/2012 06:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.341e-003 3.341e-003

Ca 1.220e-003 1.220e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.627e-006 5.627e-006

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.480

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 323

Density (g/cm3) = 0.99741

Activity of water = 1.000

Ionic strength = 5.223e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.555e-003

Total CO2 (mol/kg) = 3.555e-003

Temperature (deg C) = 24.450

Electrical balance (eq) = -1.399e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.02

Iterations = 6

Total H = 1.110157e+002

Total O = 5.551712e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.6981 0.7498

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.135e-007 2.899e-007 -6.504 -6.538 -0.034

H+ 3.551e-008 3.311e-008 -7.450 -7.480 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.555e-003

HCO3- 3.265e-003 3.029e-003 -2.486 -2.519 -0.033

CO2 2.268e-004 2.271e-004 -3.644 -3.644 0.001

CaHCO3+ 3.564e-005 3.306e-005 -4.448 -4.481 -0.033

MgHCO3+ 1.409e-005 1.304e-005 -4.851 -4.885 -0.033

CaCO3 6.074e-006 6.082e-006 -5.216 -5.216 0.001

CO3-2 5.727e-006 4.242e-006 -5.242 -5.372 -0.130

MgCO3 1.479e-006 1.481e-006 -5.830 -5.829 0.001

NaHCO3 1.574e-008 1.576e-008 -7.803 -7.803 0.001

NaCO3- 7.677e-010 7.108e-010 -9.115 -9.148 -0.033

Ca 1.220e-003

Ca+2 1.166e-003 8.629e-004 -2.933 -3.064 -0.131

CaHCO3+ 3.564e-005 3.306e-005 -4.448 -4.481 -0.033

CaSO4 1.225e-005 1.227e-005 -4.912 -4.911 0.001

CaCO3 6.074e-006 6.082e-006 -5.216 -5.216 0.001

CaOH+ 4.671e-009 4.324e-009 -8.331 -8.364 -0.033

CaHSO4+ 2.553e-012 2.364e-012 -11.593 -11.626 -0.033

Cl 5.727e-005

Cl- 5.727e-005 5.298e-005 -4.242 -4.276 -0.034

H(0) 1.559e-026

H2 7.796e-027 7.805e-027 -26.108 -26.108 0.001

K 3.326e-006

K+ 3.324e-006 3.074e-006 -5.478 -5.512 -0.034

KSO4- 1.656e-009 1.533e-009 -8.781 -8.815 -0.033

KOH 3.215e-013 3.219e-013 -12.493 -12.492 0.001

Mg 5.184e-004

Mg+2 4.967e-004 3.690e-004 -3.304 -3.433 -0.129

MgHCO3+ 1.409e-005 1.304e-005 -4.851 -4.885 -0.033

MgSO4 6.102e-006 6.109e-006 -5.215 -5.214 0.001

MgCO3 1.479e-006 1.481e-006 -5.830 -5.829 0.001

MgOH+ 4.158e-008 3.849e-008 -7.381 -7.415 -0.033

Na 1.001e-005

Na+ 9.987e-006 9.252e-006 -5.001 -5.034 -0.033

NaHCO3 1.574e-008 1.576e-008 -7.803 -7.803 0.001

NaSO4- 3.576e-009 3.310e-009 -8.447 -8.480 -0.033

NaCO3- 7.677e-010 7.108e-010 -9.115 -9.148 -0.033

NaOH 1.844e-012 1.846e-012 -11.734 -11.734 0.001

O(0) 5.627e-006

O2 2.813e-006 2.817e-006 -5.551 -5.550 0.001

S(6) 1.154e-004

SO4-2 9.701e-005 7.163e-005 -4.013 -4.145 -0.132

CaSO4 1.225e-005 1.227e-005 -4.912 -4.911 0.001

MgSO4 6.102e-006 6.109e-006 -5.215 -5.214 0.001

NaSO4- 3.576e-009 3.310e-009 -8.447 -8.480 -0.033

KSO4- 1.656e-009 1.533e-009 -8.781 -8.815 -0.033

HSO4- 2.461e-010 2.279e-010 -9.609 -9.642 -0.033

CaHSO4+ 2.553e-012 2.364e-012 -11.593 -11.626 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite -0.10 -8.44 -8.33 CaCO3

Calcite 0.04 -8.44 -8.48 CaCO3

CO2(g) -2.18 -3.64 -1.46 CO2

Dolomite -0.16 -17.24 -17.08 CaMg(CO3)2

Gypsum -2.63 -7.21 -4.58 CaSO4:2H2O

H2(g) -22.96 -26.11 -3.15 H2

H2O(g) -1.52 -0.00 1.52 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -2.66 -5.55 -2.89 O2

Initial solution 78. 30/8/2012 07:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.352e-003 3.352e-003

Ca 1.223e-003 1.223e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 7.502e-006 7.502e-006

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.480

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 324

Density (g/cm3) = 0.99744

Activity of water = 1.000

Ionic strength = 5.235e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.566e-003

Total CO2 (mol/kg) = 3.566e-003

Temperature (deg C) = 24.360

Electrical balance (eq) = -1.428e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.06

Iterations = 6

Total H = 1.110158e+002

Total O = 5.551716e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.7368 0.7518

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.114e-007 2.880e-007 -6.507 -6.541 -0.034

H+ 3.551e-008 3.311e-008 -7.450 -7.480 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.566e-003

HCO3- 3.275e-003 3.038e-003 -2.485 -2.517 -0.033

CO2 2.277e-004 2.280e-004 -3.643 -3.642 0.001

CaHCO3+ 3.580e-005 3.321e-005 -4.446 -4.479 -0.033

MgHCO3+ 1.412e-005 1.308e-005 -4.850 -4.884 -0.034

CaCO3 6.088e-006 6.095e-006 -5.216 -5.215 0.001

CO3-2 5.735e-006 4.247e-006 -5.241 -5.372 -0.131

MgCO3 1.478e-006 1.480e-006 -5.830 -5.830 0.001

NaHCO3 1.579e-008 1.580e-008 -7.802 -7.801 0.001

NaCO3- 7.652e-010 7.083e-010 -9.116 -9.150 -0.034

Ca 1.223e-003

Ca+2 1.169e-003 8.653e-004 -2.932 -3.063 -0.131

CaHCO3+ 3.580e-005 3.321e-005 -4.446 -4.479 -0.033

CaSO4 1.227e-005 1.229e-005 -4.911 -4.910 0.001

CaCO3 6.088e-006 6.095e-006 -5.216 -5.215 0.001

CaOH+ 4.684e-009 4.336e-009 -8.329 -8.363 -0.034

CaHSO4+ 2.555e-012 2.365e-012 -11.593 -11.626 -0.034

Cl 5.727e-005

Cl- 5.727e-005 5.297e-005 -4.242 -4.276 -0.034

H(0) 1.561e-026

H2 7.803e-027 7.812e-027 -26.108 -26.107 0.001

K 3.326e-006

K+ 3.324e-006 3.074e-006 -5.478 -5.512 -0.034

KSO4- 1.652e-009 1.530e-009 -8.782 -8.815 -0.034

KOH 3.215e-013 3.219e-013 -12.493 -12.492 0.001

Mg 5.184e-004

Mg+2 4.967e-004 3.689e-004 -3.304 -3.433 -0.129

MgHCO3+ 1.412e-005 1.308e-005 -4.850 -4.884 -0.034

MgSO4 6.084e-006 6.091e-006 -5.216 -5.215 0.001

MgCO3 1.478e-006 1.480e-006 -5.830 -5.830 0.001

MgOH+ 4.123e-008 3.817e-008 -7.385 -7.418 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.252e-006 -5.001 -5.034 -0.033

NaHCO3 1.579e-008 1.580e-008 -7.802 -7.801 0.001

NaSO4- 3.572e-009 3.307e-009 -8.447 -8.481 -0.034

NaCO3- 7.652e-010 7.083e-010 -9.116 -9.150 -0.034

NaOH 1.844e-012 1.846e-012 -11.734 -11.734 0.001

O(0) 7.502e-006

O2 3.751e-006 3.756e-006 -5.426 -5.425 0.001

S(6) 1.154e-004

SO4-2 9.701e-005 7.161e-005 -4.013 -4.145 -0.132

CaSO4 1.227e-005 1.229e-005 -4.911 -4.910 0.001

MgSO4 6.084e-006 6.091e-006 -5.216 -5.215 0.001

NaSO4- 3.572e-009 3.307e-009 -8.447 -8.481 -0.034

KSO4- 1.652e-009 1.530e-009 -8.782 -8.815 -0.034

HSO4- 2.456e-010 2.274e-010 -9.610 -9.643 -0.034

CaHSO4+ 2.555e-012 2.365e-012 -11.593 -11.626 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite -0.10 -8.43 -8.33 CaCO3

Calcite 0.04 -8.43 -8.48 CaCO3

CO2(g) -2.18 -3.64 -1.46 CO2

Dolomite -0.16 -17.24 -17.08 CaMg(CO3)2

Gypsum -2.63 -7.21 -4.58 CaSO4:2H2O

H2(g) -22.96 -26.11 -3.15 H2

H2O(g) -1.53 -0.00 1.53 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -2.54 -5.43 -2.89 O2

Initial solution 79. 30/8/2012 07:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.352e-003 3.352e-003

Ca 1.223e-003 1.223e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.627e-006 5.627e-006

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.480

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 323

Density (g/cm3) = 0.99745

Activity of water = 1.000

Ionic strength = 5.235e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.566e-003

Total CO2 (mol/kg) = 3.566e-003

Temperature (deg C) = 24.310

Electrical balance (eq) = -1.428e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.06

Iterations = 6

Total H = 1.110158e+002

Total O = 5.551715e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.7097 0.7501

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.102e-007 2.869e-007 -6.508 -6.542 -0.034

H+ 3.551e-008 3.311e-008 -7.450 -7.480 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.566e-003

HCO3- 3.275e-003 3.038e-003 -2.485 -2.517 -0.033

CO2 2.279e-004 2.282e-004 -3.642 -3.642 0.001

CaHCO3+ 3.577e-005 3.318e-005 -4.446 -4.479 -0.033

MgHCO3+ 1.412e-005 1.307e-005 -4.850 -4.884 -0.034

CaCO3 6.076e-006 6.083e-006 -5.216 -5.216 0.001

CO3-2 5.730e-006 4.243e-006 -5.242 -5.372 -0.130

MgCO3 1.476e-006 1.478e-006 -5.831 -5.830 0.001

NaHCO3 1.579e-008 1.580e-008 -7.802 -7.801 0.001

NaCO3- 7.625e-010 7.058e-010 -9.118 -9.151 -0.034

Ca 1.223e-003

Ca+2 1.169e-003 8.653e-004 -2.932 -3.063 -0.131

CaHCO3+ 3.577e-005 3.318e-005 -4.446 -4.479 -0.033

CaSO4 1.227e-005 1.229e-005 -4.911 -4.911 0.001

CaCO3 6.076e-006 6.083e-006 -5.216 -5.216 0.001

CaOH+ 4.684e-009 4.336e-009 -8.329 -8.363 -0.034

CaHSO4+ 2.553e-012 2.363e-012 -11.593 -11.627 -0.034

Cl 5.727e-005

Cl- 5.727e-005 5.297e-005 -4.242 -4.276 -0.034

H(0) 1.561e-026

H2 7.807e-027 7.816e-027 -26.108 -26.107 0.001

K 3.326e-006

K+ 3.324e-006 3.074e-006 -5.478 -5.512 -0.034

KSO4- 1.651e-009 1.529e-009 -8.782 -8.816 -0.034

KOH 3.215e-013 3.219e-013 -12.493 -12.492 0.001

Mg 5.184e-004

Mg+2 4.967e-004 3.689e-004 -3.304 -3.433 -0.129

MgHCO3+ 1.412e-005 1.307e-005 -4.850 -4.884 -0.034

MgSO4 6.077e-006 6.084e-006 -5.216 -5.216 0.001

MgCO3 1.476e-006 1.478e-006 -5.831 -5.830 0.001

MgOH+ 4.105e-008 3.800e-008 -7.387 -7.420 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.252e-006 -5.001 -5.034 -0.033

NaHCO3 1.579e-008 1.580e-008 -7.802 -7.801 0.001

NaSO4- 3.572e-009 3.306e-009 -8.447 -8.481 -0.034

NaCO3- 7.625e-010 7.058e-010 -9.118 -9.151 -0.034

NaOH 1.844e-012 1.846e-012 -11.734 -11.734 0.001

O(0) 5.627e-006

O2 2.813e-006 2.817e-006 -5.551 -5.550 0.001

S(6) 1.154e-004

SO4-2 9.702e-005 7.162e-005 -4.013 -4.145 -0.132

CaSO4 1.227e-005 1.229e-005 -4.911 -4.911 0.001

MgSO4 6.077e-006 6.084e-006 -5.216 -5.216 0.001

NaSO4- 3.572e-009 3.306e-009 -8.447 -8.481 -0.034

KSO4- 1.651e-009 1.529e-009 -8.782 -8.816 -0.034

HSO4- 2.454e-010 2.271e-010 -9.610 -9.644 -0.034

CaHSO4+ 2.553e-012 2.363e-012 -11.593 -11.627 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite -0.10 -8.44 -8.33 CaCO3

Calcite 0.04 -8.44 -8.48 CaCO3

CO2(g) -2.18 -3.64 -1.46 CO2

Dolomite -0.17 -17.24 -17.07 CaMg(CO3)2

Gypsum -2.63 -7.21 -4.58 CaSO4:2H2O

H2(g) -22.96 -26.11 -3.15 H2

H2O(g) -1.53 -0.00 1.53 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -2.66 -5.55 -2.89 O2

Initial solution 80. 30/8/2012 07:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.372e-003 3.372e-003

Ca 1.231e-003 1.231e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.376e-006 4.376e-006

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.480

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 324

Density (g/cm3) = 0.99747

Activity of water = 1.000

Ionic strength = 5.259e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.588e-003

Total CO2 (mol/kg) = 3.588e-003

Temperature (deg C) = 24.240

Electrical balance (eq) = -1.485e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.13

Iterations = 6

Total H = 1.110158e+002

Total O = 5.551722e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.6883 0.7487

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.086e-007 2.853e-007 -6.511 -6.545 -0.034

H+ 3.551e-008 3.311e-008 -7.450 -7.480 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.588e-003

HCO3- 3.295e-003 3.056e-003 -2.482 -2.515 -0.033

CO2 2.294e-004 2.297e-004 -3.639 -3.639 0.001

CaHCO3+ 3.615e-005 3.352e-005 -4.442 -4.475 -0.033

MgHCO3+ 1.420e-005 1.314e-005 -4.848 -4.881 -0.034

CaCO3 6.128e-006 6.136e-006 -5.213 -5.212 0.001

CO3-2 5.759e-006 4.262e-006 -5.240 -5.370 -0.131

MgCO3 1.480e-006 1.482e-006 -5.830 -5.829 0.001

NaHCO3 1.588e-008 1.590e-008 -7.799 -7.799 0.001

NaCO3- 7.632e-010 7.064e-010 -9.117 -9.151 -0.034

Ca 1.231e-003

Ca+2 1.176e-003 8.700e-004 -2.929 -3.060 -0.131

CaHCO3+ 3.615e-005 3.352e-005 -4.442 -4.475 -0.033

CaSO4 1.232e-005 1.233e-005 -4.909 -4.909 0.001

CaCO3 6.128e-006 6.136e-006 -5.213 -5.212 0.001

CaOH+ 4.711e-009 4.360e-009 -8.327 -8.361 -0.034

CaHSO4+ 2.561e-012 2.370e-012 -11.592 -11.625 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.297e-005 -4.242 -4.276 -0.034

H(0) 1.562e-026

H2 7.812e-027 7.822e-027 -26.107 -26.107 0.001

K 3.326e-006

K+ 3.324e-006 3.074e-006 -5.478 -5.512 -0.034

KSO4- 1.648e-009 1.525e-009 -8.783 -8.817 -0.034

KOH 3.214e-013 3.218e-013 -12.493 -12.492 0.001

Mg 5.184e-004

Mg+2 4.966e-004 3.687e-004 -3.304 -3.433 -0.129

MgHCO3+ 1.420e-005 1.314e-005 -4.848 -4.881 -0.034

MgSO4 6.057e-006 6.064e-006 -5.218 -5.217 0.001

MgCO3 1.480e-006 1.482e-006 -5.830 -5.829 0.001

MgOH+ 4.076e-008 3.773e-008 -7.390 -7.423 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.250e-006 -5.001 -5.034 -0.033

NaHCO3 1.588e-008 1.590e-008 -7.799 -7.799 0.001

NaSO4- 3.567e-009 3.302e-009 -8.448 -8.481 -0.034

NaCO3- 7.632e-010 7.064e-010 -9.117 -9.151 -0.034

NaOH 1.843e-012 1.845e-012 -11.734 -11.734 0.001

O(0) 4.376e-006

O2 2.188e-006 2.191e-006 -5.660 -5.659 0.001

S(6) 1.154e-004

SO4-2 9.699e-005 7.156e-005 -4.013 -4.145 -0.132

CaSO4 1.232e-005 1.233e-005 -4.909 -4.909 0.001

MgSO4 6.057e-006 6.064e-006 -5.218 -5.217 0.001

NaSO4- 3.567e-009 3.302e-009 -8.448 -8.481 -0.034

KSO4- 1.648e-009 1.525e-009 -8.783 -8.817 -0.034

HSO4- 2.448e-010 2.266e-010 -9.611 -9.645 -0.034

CaHSO4+ 2.561e-012 2.370e-012 -11.592 -11.625 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite -0.10 -8.43 -8.33 CaCO3

Calcite 0.04 -8.43 -8.48 CaCO3

CO2(g) -2.18 -3.64 -1.46 CO2

Dolomite -0.16 -17.23 -17.07 CaMg(CO3)2

Gypsum -2.63 -7.21 -4.58 CaSO4:2H2O

H2(g) -22.96 -26.11 -3.15 H2

H2O(g) -1.53 -0.00 1.53 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -2.77 -5.66 -2.89 O2

Initial solution 81. 30/8/2012 07:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.372e-003 3.372e-003

Ca 1.231e-003 1.231e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.563e-005 1.563e-005

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.490

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 324

Density (g/cm3) = 0.99747

Activity of water = 1.000

Ionic strength = 5.259e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.583e-003

Total CO2 (mol/kg) = 3.583e-003

Temperature (deg C) = 24.240

Electrical balance (eq) = -1.485e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.13

Iterations = 6

Total H = 1.110158e+002

Total O = 5.551722e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8165 0.7562

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.158e-007 2.920e-007 -6.501 -6.535 -0.034

H+ 3.470e-008 3.236e-008 -7.460 -7.490 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.583e-003

HCO3- 3.294e-003 3.055e-003 -2.482 -2.515 -0.033

CO2 2.242e-004 2.245e-004 -3.649 -3.649 0.001

CaHCO3+ 3.613e-005 3.352e-005 -4.442 -4.475 -0.033

MgHCO3+ 1.419e-005 1.314e-005 -4.848 -4.882 -0.034

CaCO3 6.269e-006 6.277e-006 -5.203 -5.202 0.001

CO3-2 5.892e-006 4.360e-006 -5.230 -5.360 -0.131

MgCO3 1.514e-006 1.516e-006 -5.820 -5.819 0.001

NaHCO3 1.587e-008 1.589e-008 -7.799 -7.799 0.001

NaCO3- 7.808e-010 7.227e-010 -9.107 -9.141 -0.034

Ca 1.231e-003

Ca+2 1.176e-003 8.699e-004 -2.930 -3.061 -0.131

CaHCO3+ 3.613e-005 3.352e-005 -4.442 -4.475 -0.033

CaSO4 1.232e-005 1.233e-005 -4.909 -4.909 0.001

CaCO3 6.269e-006 6.277e-006 -5.203 -5.202 0.001

CaOH+ 4.820e-009 4.461e-009 -8.317 -8.351 -0.034

CaHSO4+ 2.502e-012 2.316e-012 -11.602 -11.635 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.297e-005 -4.242 -4.276 -0.034

H(0) 1.492e-026

H2 7.461e-027 7.470e-027 -26.127 -26.127 0.001

K 3.326e-006

K+ 3.324e-006 3.074e-006 -5.478 -5.512 -0.034

KSO4- 1.648e-009 1.525e-009 -8.783 -8.817 -0.034

KOH 3.289e-013 3.293e-013 -12.483 -12.482 0.001

Mg 5.184e-004

Mg+2 4.966e-004 3.686e-004 -3.304 -3.433 -0.129

MgHCO3+ 1.419e-005 1.314e-005 -4.848 -4.882 -0.034

MgSO4 6.056e-006 6.064e-006 -5.218 -5.217 0.001

MgCO3 1.514e-006 1.516e-006 -5.820 -5.819 0.001

MgOH+ 4.171e-008 3.861e-008 -7.380 -7.413 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.250e-006 -5.001 -5.034 -0.033

NaHCO3 1.587e-008 1.589e-008 -7.799 -7.799 0.001

NaSO4- 3.567e-009 3.302e-009 -8.448 -8.481 -0.034

NaCO3- 7.808e-010 7.227e-010 -9.107 -9.141 -0.034

NaOH 1.886e-012 1.888e-012 -11.724 -11.724 0.001

O(0) 1.563e-005

O2 7.815e-006 7.824e-006 -5.107 -5.107 0.001

S(6) 1.154e-004

SO4-2 9.699e-005 7.156e-005 -4.013 -4.145 -0.132

CaSO4 1.232e-005 1.233e-005 -4.909 -4.909 0.001

MgSO4 6.056e-006 6.064e-006 -5.218 -5.217 0.001

NaSO4- 3.567e-009 3.302e-009 -8.448 -8.481 -0.034

KSO4- 1.648e-009 1.525e-009 -8.783 -8.817 -0.034

HSO4- 2.393e-010 2.214e-010 -9.621 -9.655 -0.034

CaHSO4+ 2.502e-012 2.316e-012 -11.602 -11.635 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite -0.09 -8.42 -8.33 CaCO3

Calcite 0.05 -8.42 -8.48 CaCO3

CO2(g) -2.19 -3.65 -1.46 CO2

Dolomite -0.14 -17.21 -17.07 CaMg(CO3)2

Gypsum -2.63 -7.21 -4.58 CaSO4:2H2O

H2(g) -22.98 -26.13 -3.15 H2

H2O(g) -1.53 -0.00 1.53 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -2.22 -5.11 -2.89 O2

Initial solution 82. 30/8/2012 08:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.383e-003 3.383e-003

Ca 1.235e-003 1.235e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 2.313e-005 2.313e-005

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.500

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 325

Density (g/cm3) = 0.99745

Activity of water = 1.000

Ionic strength = 5.271e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.588e-003

Total CO2 (mol/kg) = 3.588e-003

Temperature (deg C) = 24.310

Electrical balance (eq) = -1.513e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.17

Iterations = 6

Total H = 1.110158e+002

Total O = 5.551725e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8432 0.7580

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.249e-007 3.004e-007 -6.488 -6.522 -0.034

H+ 3.392e-008 3.162e-008 -7.470 -7.500 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.588e-003

HCO3- 3.304e-003 3.064e-003 -2.481 -2.514 -0.033

CO2 2.195e-004 2.197e-004 -3.659 -3.658 0.001

CaHCO3+ 3.637e-005 3.373e-005 -4.439 -4.472 -0.033

MgHCO3+ 1.423e-005 1.317e-005 -4.847 -4.880 -0.034

CaCO3 6.467e-006 6.474e-006 -5.189 -5.189 0.001

CO3-2 6.056e-006 4.480e-006 -5.218 -5.349 -0.131

MgCO3 1.557e-006 1.559e-006 -5.808 -5.807 0.001

NaHCO3 1.592e-008 1.594e-008 -7.798 -7.798 0.001

NaCO3- 8.052e-010 7.452e-010 -9.094 -9.128 -0.034

Ca 1.235e-003

Ca+2 1.179e-003 8.721e-004 -2.928 -3.059 -0.131

CaHCO3+ 3.637e-005 3.373e-005 -4.439 -4.472 -0.033

CaSO4 1.235e-005 1.236e-005 -4.908 -4.908 0.001

CaCO3 6.467e-006 6.474e-006 -5.189 -5.189 0.001

CaOH+ 4.945e-009 4.576e-009 -8.306 -8.339 -0.034

CaHSO4+ 2.454e-012 2.271e-012 -11.610 -11.644 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.296e-005 -4.242 -4.276 -0.034

H(0) 1.424e-026

H2 7.120e-027 7.128e-027 -26.148 -26.147 0.001

K 3.326e-006

K+ 3.324e-006 3.074e-006 -5.478 -5.512 -0.034

KSO4- 1.649e-009 1.526e-009 -8.783 -8.816 -0.034

KOH 3.366e-013 3.370e-013 -12.473 -12.472 0.001

Mg 5.184e-004

Mg+2 4.965e-004 3.685e-004 -3.304 -3.434 -0.130

MgHCO3+ 1.423e-005 1.317e-005 -4.847 -4.880 -0.034

MgSO4 6.060e-006 6.068e-006 -5.218 -5.217 0.001

MgCO3 1.557e-006 1.559e-006 -5.808 -5.807 0.001

MgOH+ 4.294e-008 3.974e-008 -7.367 -7.401 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.249e-006 -5.001 -5.034 -0.033

NaHCO3 1.592e-008 1.594e-008 -7.798 -7.798 0.001

NaSO4- 3.566e-009 3.301e-009 -8.448 -8.481 -0.034

NaCO3- 8.052e-010 7.452e-010 -9.094 -9.128 -0.034

NaOH 1.930e-012 1.932e-012 -11.714 -11.714 0.001

O(0) 2.313e-005

O2 1.157e-005 1.158e-005 -4.937 -4.936 0.001

S(6) 1.154e-004

SO4-2 9.696e-005 7.151e-005 -4.013 -4.146 -0.132

CaSO4 1.235e-005 1.236e-005 -4.908 -4.908 0.001

MgSO4 6.060e-006 6.068e-006 -5.218 -5.217 0.001

NaSO4- 3.566e-009 3.301e-009 -8.448 -8.481 -0.034

KSO4- 1.649e-009 1.526e-009 -8.783 -8.816 -0.034

HSO4- 2.340e-010 2.166e-010 -9.631 -9.664 -0.034

CaHSO4+ 2.454e-012 2.271e-012 -11.610 -11.644 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite -0.08 -8.41 -8.33 CaCO3

Calcite 0.07 -8.41 -8.48 CaCO3

CO2(g) -2.20 -3.66 -1.46 CO2

Dolomite -0.12 -17.19 -17.07 CaMg(CO3)2

Gypsum -2.62 -7.21 -4.58 CaSO4:2H2O

H2(g) -23.00 -26.15 -3.15 H2

H2O(g) -1.53 -0.00 1.53 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -2.05 -4.94 -2.89 O2

Initial solution 83. 30/8/2012 08:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.383e-003 3.383e-003

Ca 1.235e-003 1.235e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.064e-005 4.064e-005

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.530

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 326

Density (g/cm3) = 0.99744

Activity of water = 1.000

Ionic strength = 5.269e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.572e-003

Total CO2 (mol/kg) = 3.572e-003

Temperature (deg C) = 24.350

Electrical balance (eq) = -1.513e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.17

Iterations = 6

Total H = 1.110158e+002

Total O = 5.551723e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8711 0.7597

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.492e-007 3.229e-007 -6.457 -6.491 -0.034

H+ 3.165e-008 2.951e-008 -7.500 -7.530 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.572e-003

HCO3- 3.302e-003 3.062e-003 -2.481 -2.514 -0.033

CO2 2.046e-004 2.048e-004 -3.689 -3.689 0.001

CaHCO3+ 3.635e-005 3.371e-005 -4.439 -4.472 -0.033

MgHCO3+ 1.422e-005 1.316e-005 -4.847 -4.881 -0.034

CaCO3 6.933e-006 6.942e-006 -5.159 -5.159 0.001

CO3-2 6.491e-006 4.802e-006 -5.188 -5.319 -0.131

MgCO3 1.669e-006 1.671e-006 -5.778 -5.777 0.001

NaHCO3 1.591e-008 1.593e-008 -7.798 -7.798 0.001

NaCO3- 8.647e-010 8.003e-010 -9.063 -9.097 -0.034

Ca 1.235e-003

Ca+2 1.179e-003 8.717e-004 -2.928 -3.060 -0.131

CaHCO3+ 3.635e-005 3.371e-005 -4.439 -4.472 -0.033

CaSO4 1.235e-005 1.236e-005 -4.908 -4.908 0.001

CaCO3 6.933e-006 6.942e-006 -5.159 -5.159 0.001

CaOH+ 5.296e-009 4.902e-009 -8.276 -8.310 -0.034

CaHSO4+ 2.291e-012 2.120e-012 -11.640 -11.674 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.296e-005 -4.242 -4.276 -0.034

H(0) 1.240e-026

H2 6.199e-027 6.206e-027 -26.208 -26.207 0.001

K 3.326e-006

K+ 3.324e-006 3.074e-006 -5.478 -5.512 -0.034

KSO4- 1.650e-009 1.527e-009 -8.783 -8.816 -0.034

KOH 3.606e-013 3.611e-013 -12.443 -12.442 0.001

Mg 5.184e-004

Mg+2 4.964e-004 3.684e-004 -3.304 -3.434 -0.130

MgHCO3+ 1.422e-005 1.316e-005 -4.847 -4.881 -0.034

MgSO4 6.065e-006 6.072e-006 -5.217 -5.217 0.001

MgCO3 1.669e-006 1.671e-006 -5.778 -5.777 0.001

MgOH+ 4.617e-008 4.273e-008 -7.336 -7.369 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.249e-006 -5.001 -5.034 -0.033

NaHCO3 1.591e-008 1.593e-008 -7.798 -7.798 0.001

NaSO4- 3.567e-009 3.301e-009 -8.448 -8.481 -0.034

NaCO3- 8.647e-010 8.003e-010 -9.063 -9.097 -0.034

NaOH 2.068e-012 2.070e-012 -11.684 -11.684 0.001

O(0) 4.064e-005

O2 2.032e-005 2.034e-005 -4.692 -4.692 0.001

S(6) 1.154e-004

SO4-2 9.695e-005 7.151e-005 -4.013 -4.146 -0.132

CaSO4 1.235e-005 1.236e-005 -4.908 -4.908 0.001

MgSO4 6.065e-006 6.072e-006 -5.217 -5.217 0.001

NaSO4- 3.567e-009 3.301e-009 -8.448 -8.481 -0.034

KSO4- 1.650e-009 1.527e-009 -8.783 -8.816 -0.034

HSO4- 2.186e-010 2.023e-010 -9.660 -9.694 -0.034

CaHSO4+ 2.291e-012 2.120e-012 -11.640 -11.674 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite -0.05 -8.38 -8.33 CaCO3

Calcite 0.10 -8.38 -8.48 CaCO3

CO2(g) -2.23 -3.69 -1.46 CO2

Dolomite -0.06 -17.13 -17.07 CaMg(CO3)2

Gypsum -2.62 -7.21 -4.58 CaSO4:2H2O

H2(g) -23.06 -26.21 -3.15 H2

H2O(g) -1.53 -0.00 1.53 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -1.80 -4.69 -2.89 O2

Initial solution 84. 30/8/2012 08:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.383e-003 3.383e-003

Ca 1.235e-003 1.235e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.814e-005 3.814e-005

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.540

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 326

Density (g/cm3) = 0.99743

Activity of water = 1.000

Ionic strength = 5.269e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.567e-003

Total CO2 (mol/kg) = 3.567e-003

Temperature (deg C) = 24.380

Electrical balance (eq) = -1.513e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.17

Iterations = 6

Total H = 1.110158e+002

Total O = 5.551722e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8517 0.7587

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.582e-007 3.311e-007 -6.446 -6.480 -0.034

H+ 3.093e-008 2.884e-008 -7.510 -7.540 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.567e-003

HCO3- 3.301e-003 3.061e-003 -2.481 -2.514 -0.033

CO2 1.998e-004 2.001e-004 -3.699 -3.699 0.001

CaHCO3+ 3.636e-005 3.372e-005 -4.439 -4.472 -0.033

MgHCO3+ 1.422e-005 1.316e-005 -4.847 -4.881 -0.034

CaCO3 7.101e-006 7.109e-006 -5.149 -5.148 0.001

CO3-2 6.644e-006 4.916e-006 -5.178 -5.308 -0.131

MgCO3 1.709e-006 1.711e-006 -5.767 -5.767 0.001

NaHCO3 1.590e-008 1.592e-008 -7.799 -7.798 0.001

NaCO3- 8.865e-010 8.205e-010 -9.052 -9.086 -0.034

Ca 1.235e-003

Ca+2 1.179e-003 8.716e-004 -2.929 -3.060 -0.131

CaHCO3+ 3.636e-005 3.372e-005 -4.439 -4.472 -0.033

CaSO4 1.235e-005 1.236e-005 -4.908 -4.908 0.001

CaCO3 7.101e-006 7.109e-006 -5.149 -5.148 0.001

CaOH+ 5.419e-009 5.015e-009 -8.266 -8.300 -0.034

CaHSO4+ 2.240e-012 2.073e-012 -11.650 -11.683 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.296e-005 -4.242 -4.276 -0.034

H(0) 1.184e-026

H2 5.918e-027 5.925e-027 -26.228 -26.227 0.001

K 3.326e-006

K+ 3.324e-006 3.074e-006 -5.478 -5.512 -0.034

KSO4- 1.651e-009 1.528e-009 -8.782 -8.816 -0.034

KOH 3.690e-013 3.695e-013 -12.433 -12.432 0.001

Mg 5.184e-004

Mg+2 4.964e-004 3.683e-004 -3.304 -3.434 -0.130

MgHCO3+ 1.422e-005 1.316e-005 -4.847 -4.881 -0.034

MgSO4 6.069e-006 6.076e-006 -5.217 -5.216 0.001

MgCO3 1.709e-006 1.711e-006 -5.767 -5.767 0.001

MgOH+ 4.737e-008 4.384e-008 -7.325 -7.358 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.249e-006 -5.001 -5.034 -0.033

NaHCO3 1.590e-008 1.592e-008 -7.799 -7.798 0.001

NaSO4- 3.568e-009 3.302e-009 -8.448 -8.481 -0.034

NaCO3- 8.865e-010 8.205e-010 -9.052 -9.086 -0.034

NaOH 2.116e-012 2.119e-012 -11.674 -11.674 0.001

O(0) 3.814e-005

O2 1.907e-005 1.909e-005 -4.720 -4.719 0.001

S(6) 1.154e-004

SO4-2 9.695e-005 7.151e-005 -4.013 -4.146 -0.132

CaSO4 1.235e-005 1.236e-005 -4.908 -4.908 0.001

MgSO4 6.069e-006 6.076e-006 -5.217 -5.216 0.001

NaSO4- 3.568e-009 3.302e-009 -8.448 -8.481 -0.034

KSO4- 1.651e-009 1.528e-009 -8.782 -8.816 -0.034

HSO4- 2.137e-010 1.978e-010 -9.670 -9.704 -0.034

CaHSO4+ 2.240e-012 2.073e-012 -11.650 -11.683 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite -0.04 -8.37 -8.33 CaCO3

Calcite 0.11 -8.37 -8.48 CaCO3

CO2(g) -2.24 -3.70 -1.46 CO2

Dolomite -0.03 -17.11 -17.08 CaMg(CO3)2

Gypsum -2.62 -7.21 -4.58 CaSO4:2H2O

H2(g) -23.08 -26.23 -3.15 H2

H2O(g) -1.53 -0.00 1.53 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -1.83 -4.72 -2.89 O2

Initial solution 85. 30/8/2012 08:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.372e-003 3.372e-003

Ca 1.231e-003 1.231e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.189e-005 4.189e-005

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.570

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 326

Density (g/cm3) = 0.99740

Activity of water = 1.000

Ionic strength = 5.255e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.541e-003

Total CO2 (mol/kg) = 3.541e-003

Temperature (deg C) = 24.520

Electrical balance (eq) = -1.485e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.13

Iterations = 6

Total H = 1.110158e+002

Total O = 5.551716e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8202 0.7572

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.879e-007 3.586e-007 -6.411 -6.445 -0.034

H+ 2.887e-008 2.692e-008 -7.540 -7.570 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.541e-003

HCO3- 3.288e-003 3.050e-003 -2.483 -2.516 -0.033

CO2 1.855e-004 1.857e-004 -3.732 -3.731 0.001

CaHCO3+ 3.618e-005 3.356e-005 -4.441 -4.474 -0.033

MgHCO3+ 1.417e-005 1.312e-005 -4.849 -4.882 -0.034

CaCO3 7.599e-006 7.609e-006 -5.119 -5.119 0.001

CO3-2 7.112e-006 5.263e-006 -5.148 -5.279 -0.131

MgCO3 1.834e-006 1.836e-006 -5.737 -5.736 0.001

NaHCO3 1.585e-008 1.587e-008 -7.800 -7.800 0.001

NaCO3- 9.559e-010 8.848e-010 -9.020 -9.053 -0.034

Ca 1.231e-003

Ca+2 1.175e-003 8.689e-004 -2.930 -3.061 -0.131

CaHCO3+ 3.618e-005 3.356e-005 -4.441 -4.474 -0.033

CaSO4 1.233e-005 1.234e-005 -4.909 -4.909 0.001

CaCO3 7.599e-006 7.609e-006 -5.119 -5.119 0.001

CaOH+ 5.788e-009 5.357e-009 -8.237 -8.271 -0.034

CaHSO4+ 2.090e-012 1.935e-012 -11.680 -11.713 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.297e-005 -4.242 -4.276 -0.034

H(0) 1.029e-026

H2 5.147e-027 5.153e-027 -26.288 -26.288 0.001

K 3.326e-006

K+ 3.324e-006 3.074e-006 -5.478 -5.512 -0.034

KSO4- 1.655e-009 1.532e-009 -8.781 -8.815 -0.034

KOH 3.955e-013 3.959e-013 -12.403 -12.402 0.001

Mg 5.184e-004

Mg+2 4.963e-004 3.684e-004 -3.304 -3.434 -0.129

MgHCO3+ 1.417e-005 1.312e-005 -4.849 -4.882 -0.034

MgSO4 6.093e-006 6.100e-006 -5.215 -5.215 0.001

MgCO3 1.834e-006 1.836e-006 -5.737 -5.736 0.001

MgOH+ 5.140e-008 4.757e-008 -7.289 -7.323 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.250e-006 -5.001 -5.034 -0.033

NaHCO3 1.585e-008 1.587e-008 -7.800 -7.800 0.001

NaSO4- 3.572e-009 3.306e-009 -8.447 -8.481 -0.034

NaCO3- 9.559e-010 8.848e-010 -9.020 -9.053 -0.034

NaOH 2.268e-012 2.270e-012 -11.644 -11.644 0.001

O(0) 4.189e-005

O2 2.094e-005 2.097e-005 -4.679 -4.678 0.001

S(6) 1.154e-004

SO4-2 9.695e-005 7.152e-005 -4.013 -4.146 -0.132

CaSO4 1.233e-005 1.234e-005 -4.909 -4.909 0.001

MgSO4 6.093e-006 6.100e-006 -5.215 -5.215 0.001

NaSO4- 3.572e-009 3.306e-009 -8.447 -8.481 -0.034

KSO4- 1.655e-009 1.532e-009 -8.781 -8.815 -0.034

HSO4- 2.001e-010 1.852e-010 -9.699 -9.732 -0.034

CaHSO4+ 2.090e-012 1.935e-012 -11.680 -11.713 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite -0.01 -8.34 -8.33 CaCO3

Calcite 0.14 -8.34 -8.48 CaCO3

CO2(g) -2.27 -3.73 -1.46 CO2

Dolomite 0.03 -17.05 -17.08 CaMg(CO3)2

Gypsum -2.63 -7.21 -4.58 CaSO4:2H2O

H2(g) -23.14 -26.29 -3.15 H2

H2O(g) -1.52 -0.00 1.52 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -1.79 -4.68 -2.89 O2

Initial solution 86. 30/8/2012 09:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.372e-003 3.372e-003

Ca 1.231e-003 1.231e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 8.690e-005 8.690e-005

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.610

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 327

Density (g/cm3) = 0.99736

Activity of water = 1.000

Ionic strength = 5.253e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.522e-003

Total CO2 (mol/kg) = 3.522e-003

Temperature (deg C) = 24.680

Electrical balance (eq) = -1.485e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.13

Iterations = 7

Total H = 1.110158e+002

Total O = 5.551716e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8462 0.7591

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 4.305e-007 3.980e-007 -6.366 -6.400 -0.034

H+ 2.633e-008 2.455e-008 -7.580 -7.610 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.522e-003

HCO3- 3.285e-003 3.047e-003 -2.483 -2.516 -0.033

CO2 1.686e-004 1.688e-004 -3.773 -3.773 0.001

CaHCO3+ 3.621e-005 3.359e-005 -4.441 -4.474 -0.033

MgHCO3+ 1.416e-005 1.311e-005 -4.849 -4.882 -0.034

CaCO3 8.372e-006 8.382e-006 -5.077 -5.077 0.001

CO3-2 7.815e-006 5.783e-006 -5.107 -5.238 -0.131

MgCO3 2.020e-006 2.022e-006 -5.695 -5.694 0.001

NaHCO3 1.583e-008 1.585e-008 -7.801 -7.800 0.001

NaCO3- 1.059e-009 9.802e-010 -8.975 -9.009 -0.034

Ca 1.231e-003

Ca+2 1.174e-003 8.682e-004 -2.930 -3.061 -0.131

CaHCO3+ 3.621e-005 3.359e-005 -4.441 -4.474 -0.033

CaSO4 1.233e-005 1.235e-005 -4.909 -4.908 0.001

CaCO3 8.372e-006 8.382e-006 -5.077 -5.077 0.001

CaOH+ 6.342e-009 5.869e-009 -8.198 -8.231 -0.034

CaHSO4+ 1.911e-012 1.769e-012 -11.719 -11.752 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.296e-005 -4.242 -4.276 -0.034

H(0) 8.549e-027

H2 4.274e-027 4.279e-027 -26.369 -26.369 0.001

K 3.326e-006

K+ 3.324e-006 3.074e-006 -5.478 -5.512 -0.034

KSO4- 1.659e-009 1.536e-009 -8.780 -8.814 -0.034

KOH 4.336e-013 4.341e-013 -12.363 -12.362 0.001

Mg 5.184e-004

Mg+2 4.961e-004 3.682e-004 -3.304 -3.434 -0.129

MgHCO3+ 1.416e-005 1.311e-005 -4.849 -4.882 -0.034

MgSO4 6.114e-006 6.121e-006 -5.214 -5.213 0.001

MgCO3 2.020e-006 2.022e-006 -5.695 -5.694 0.001

MgOH+ 5.716e-008 5.290e-008 -7.243 -7.277 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.250e-006 -5.001 -5.034 -0.033

NaHCO3 1.583e-008 1.585e-008 -7.801 -7.800 0.001

NaSO4- 3.574e-009 3.308e-009 -8.447 -8.480 -0.034

NaCO3- 1.059e-009 9.802e-010 -8.975 -9.009 -0.034

NaOH 2.486e-012 2.489e-012 -11.604 -11.604 0.001

O(0) 8.690e-005

O2 4.345e-005 4.350e-005 -4.362 -4.361 0.001

S(6) 1.154e-004

SO4-2 9.692e-005 7.150e-005 -4.014 -4.146 -0.132

CaSO4 1.233e-005 1.235e-005 -4.909 -4.908 0.001

MgSO4 6.114e-006 6.121e-006 -5.214 -5.213 0.001

NaSO4- 3.574e-009 3.308e-009 -8.447 -8.480 -0.034

KSO4- 1.659e-009 1.536e-009 -8.780 -8.814 -0.034

HSO4- 1.831e-010 1.695e-010 -9.737 -9.771 -0.034

CaHSO4+ 1.911e-012 1.769e-012 -11.719 -11.752 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite 0.03 -8.30 -8.33 CaCO3

Calcite 0.18 -8.30 -8.48 CaCO3

CO2(g) -2.31 -3.77 -1.46 CO2

Dolomite 0.11 -16.97 -17.08 CaMg(CO3)2

Gypsum -2.63 -7.21 -4.58 CaSO4:2H2O

H2(g) -23.22 -26.37 -3.15 H2

H2O(g) -1.52 -0.00 1.52 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -1.47 -4.36 -2.89 O2

Initial solution 87. 30/8/2012 09:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.372e-003 3.372e-003

Ca 1.231e-003 1.231e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.557e-004 1.557e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.660

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 328

Density (g/cm3) = 0.99732

Activity of water = 1.000

Ionic strength = 5.250e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.501e-003

Total CO2 (mol/kg) = 3.501e-003

Temperature (deg C) = 24.830

Electrical balance (eq) = -1.485e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.14

Iterations = 7

Total H = 1.110158e+002

Total O = 5.551719e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.8470 0.7595

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 4.885e-007 4.517e-007 -6.311 -6.345 -0.034

H+ 2.346e-008 2.188e-008 -7.630 -7.660 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.501e-003

HCO3- 3.280e-003 3.043e-003 -2.484 -2.517 -0.033

CO2 1.498e-004 1.500e-004 -3.824 -3.824 0.001

CaHCO3+ 3.621e-005 3.359e-005 -4.441 -4.474 -0.033

MgHCO3+ 1.414e-005 1.309e-005 -4.849 -4.883 -0.034

CaCO3 9.428e-006 9.440e-006 -5.026 -5.025 0.001

CO3-2 8.783e-006 6.500e-006 -5.056 -5.187 -0.131

MgCO3 2.274e-006 2.277e-006 -5.643 -5.643 0.001

NaHCO3 1.581e-008 1.583e-008 -7.801 -7.801 0.001

NaCO3- 1.199e-009 1.110e-009 -8.921 -8.955 -0.034

Ca 1.231e-003

Ca+2 1.173e-003 8.675e-004 -2.931 -3.062 -0.131

CaHCO3+ 3.621e-005 3.359e-005 -4.441 -4.474 -0.033

CaSO4 1.234e-005 1.235e-005 -4.909 -4.908 0.001

CaCO3 9.428e-006 9.440e-006 -5.026 -5.025 0.001

CaOH+ 7.109e-009 6.580e-009 -8.148 -8.182 -0.034

CaHSO4+ 1.707e-012 1.580e-012 -11.768 -11.801 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.297e-005 -4.242 -4.276 -0.034

H(0) 6.780e-027

H2 3.390e-027 3.394e-027 -26.470 -26.469 0.001

K 3.326e-006

K+ 3.324e-006 3.074e-006 -5.478 -5.512 -0.034

KSO4- 1.663e-009 1.539e-009 -8.779 -8.813 -0.034

KOH 4.865e-013 4.871e-013 -12.313 -12.312 0.001

Mg 5.184e-004

Mg+2 4.958e-004 3.680e-004 -3.305 -3.434 -0.129

MgHCO3+ 1.414e-005 1.309e-005 -4.849 -4.883 -0.034

MgSO4 6.133e-006 6.140e-006 -5.212 -5.212 0.001

MgCO3 2.274e-006 2.277e-006 -5.643 -5.643 0.001

MgOH+ 6.497e-008 6.014e-008 -7.187 -7.221 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.250e-006 -5.001 -5.034 -0.033

NaHCO3 1.581e-008 1.583e-008 -7.801 -7.801 0.001

NaSO4- 3.577e-009 3.310e-009 -8.447 -8.480 -0.034

NaCO3- 1.199e-009 1.110e-009 -8.921 -8.955 -0.034

NaOH 2.790e-012 2.793e-012 -11.554 -11.554 0.001

O(0) 1.557e-004

O2 7.783e-005 7.793e-005 -4.109 -4.108 0.001

S(6) 1.154e-004

SO4-2 9.690e-005 7.149e-005 -4.014 -4.146 -0.132

CaSO4 1.234e-005 1.235e-005 -4.909 -4.908 0.001

MgSO4 6.133e-006 6.140e-006 -5.212 -5.212 0.001

NaSO4- 3.577e-009 3.310e-009 -8.447 -8.480 -0.034

KSO4- 1.663e-009 1.539e-009 -8.779 -8.813 -0.034

HSO4- 1.637e-010 1.515e-010 -9.786 -9.820 -0.034

CaHSO4+ 1.707e-012 1.580e-012 -11.768 -11.801 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite 0.09 -8.25 -8.33 CaCO3

Calcite 0.23 -8.25 -8.48 CaCO3

CO2(g) -2.36 -3.82 -1.47 CO2

Dolomite 0.22 -16.87 -17.09 CaMg(CO3)2

Gypsum -2.63 -7.21 -4.58 CaSO4:2H2O

H2(g) -23.32 -26.47 -3.15 H2

H2O(g) -1.51 -0.00 1.51 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -1.22 -4.11 -2.89 O2

Initial solution 88. 30/8/2012 09:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.362e-003 3.362e-003

Ca 1.227e-003 1.227e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 2.488e-004 2.488e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.750

pe = 4.000

Specific Conductance (uS/cm, 24 oC) = 328

Density (g/cm3) = 0.99730

Activity of water = 1.000

Ionic strength = 5.232e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.457e-003

Total CO2 (mol/kg) = 3.457e-003

Temperature (deg C) = 24.930

Electrical balance (eq) = -1.454e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.10

Iterations = 7

Total H = 1.110157e+002

Total O = 5.551718e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.7997 0.7570

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 6.055e-007 5.599e-007 -6.218 -6.252 -0.034

H+ 1.907e-008 1.778e-008 -7.720 -7.750 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.457e-003

HCO3- 3.261e-003 3.025e-003 -2.487 -2.519 -0.033

CO2 1.209e-004 1.211e-004 -3.918 -3.917 0.001

CaHCO3+ 3.590e-005 3.330e-005 -4.445 -4.478 -0.033

MgHCO3+ 1.406e-005 1.301e-005 -4.852 -4.886 -0.034

CaCO3 1.153e-005 1.154e-005 -4.938 -4.938 0.001

CO3-2 1.076e-005 7.966e-006 -4.968 -5.099 -0.131

MgCO3 2.790e-006 2.793e-006 -5.554 -5.554 0.001

NaHCO3 1.572e-008 1.574e-008 -7.804 -7.803 0.001

NaCO3- 1.477e-009 1.367e-009 -8.831 -8.864 -0.034

Ca 1.227e-003

Ca+2 1.167e-003 8.637e-004 -2.933 -3.064 -0.131

CaHCO3+ 3.590e-005 3.330e-005 -4.445 -4.478 -0.033

CaSO4 1.230e-005 1.232e-005 -4.910 -4.909 0.001

CaCO3 1.153e-005 1.154e-005 -4.938 -4.938 0.001

CaOH+ 8.708e-009 8.060e-009 -8.060 -8.094 -0.034

CaHSO4+ 1.385e-012 1.282e-012 -11.858 -11.892 -0.034

Cl 5.728e-005

Cl- 5.728e-005 5.297e-005 -4.242 -4.276 -0.034

H(0) 4.475e-027

H2 2.238e-027 2.240e-027 -26.650 -26.650 0.001

K 3.326e-006

K+ 3.324e-006 3.074e-006 -5.478 -5.512 -0.034

KSO4- 1.667e-009 1.543e-009 -8.778 -8.812 -0.034

KOH 5.986e-013 5.993e-013 -12.223 -12.222 0.001

Mg 5.184e-004

Mg+2 4.953e-004 3.678e-004 -3.305 -3.434 -0.129

MgHCO3+ 1.406e-005 1.301e-005 -4.852 -4.886 -0.034

MgSO4 6.149e-006 6.156e-006 -5.211 -5.211 0.001

MgCO3 2.790e-006 2.793e-006 -5.554 -5.554 0.001

MgOH+ 8.061e-008 7.462e-008 -7.094 -7.127 -0.034

Na 1.001e-005

Na+ 9.987e-006 9.251e-006 -5.001 -5.034 -0.033

NaHCO3 1.572e-008 1.574e-008 -7.804 -7.803 0.001

NaSO4- 3.581e-009 3.315e-009 -8.446 -8.480 -0.034

NaCO3- 1.477e-009 1.367e-009 -8.831 -8.864 -0.034

NaOH 3.432e-012 3.437e-012 -11.464 -11.464 0.001

O(0) 2.488e-004

O2 1.244e-004 1.246e-004 -3.905 -3.905 0.001

S(6) 1.154e-004

SO4-2 9.691e-005 7.153e-005 -4.014 -4.146 -0.132

CaSO4 1.230e-005 1.232e-005 -4.910 -4.909 0.001

MgSO4 6.149e-006 6.156e-006 -5.211 -5.211 0.001

NaSO4- 3.581e-009 3.315e-009 -8.446 -8.480 -0.034

KSO4- 1.667e-009 1.543e-009 -8.778 -8.812 -0.034

HSO4- 1.334e-010 1.235e-010 -9.875 -9.908 -0.034

CaHSO4+ 1.385e-012 1.282e-012 -11.858 -11.892 -0.034

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite 0.17 -8.16 -8.34 CaCO3

Calcite 0.32 -8.16 -8.48 CaCO3

CO2(g) -2.45 -3.92 -1.47 CO2

Dolomite 0.39 -16.70 -17.09 CaMg(CO3)2

Gypsum -2.63 -7.21 -4.58 CaSO4:2H2O

H2(g) -23.50 -26.65 -3.15 H2

H2O(g) -1.51 -0.00 1.51 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -1.01 -3.90 -2.89 O2

Initial solution 89. 30/8/2012 09:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.352e-003 3.352e-003

Ca 1.223e-003 1.223e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.251e-004 3.251e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 7.850

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 327

Density (g/cm3) = 0.99727

Activity of water = 1.000

Ionic strength = 5.212e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.415e-003

Total CO2 (mol/kg) = 3.415e-003

Temperature (deg C) = 25.030

Electrical balance (eq) = -1.428e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.07

Iterations = 7

Total H = 1.110157e+002

Total O = 5.551715e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.7204 0.7526

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 7.680e-007 7.103e-007 -6.115 -6.149 -0.034

H+ 1.515e-008 1.413e-008 -7.820 -7.850 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.415e-003

HCO3- 3.239e-003 3.004e-003 -2.490 -2.522 -0.033

CO2 9.527e-005 9.539e-005 -4.021 -4.021 0.001

CaHCO3+ 3.553e-005 3.296e-005 -4.449 -4.482 -0.033

CaCO3 1.440e-005 1.442e-005 -4.842 -4.841 0.001

MgHCO3+ 1.396e-005 1.292e-005 -4.855 -4.889 -0.033

CO3-2 1.348e-005 9.981e-006 -4.870 -5.001 -0.130

MgCO3 3.497e-006 3.502e-006 -5.456 -5.456 0.001

NaHCO3 1.561e-008 1.563e-008 -7.807 -7.806 0.001

NaCO3- 1.860e-009 1.722e-009 -8.730 -8.764 -0.033

Ca 1.223e-003

Ca+2 1.161e-003 8.595e-004 -2.935 -3.066 -0.131

CaHCO3+ 3.553e-005 3.296e-005 -4.449 -4.482 -0.033

CaCO3 1.440e-005 1.442e-005 -4.842 -4.841 0.001

CaSO4 1.226e-005 1.228e-005 -4.911 -4.911 0.001

CaOH+ 1.091e-008 1.010e-008 -7.962 -7.996 -0.033

CaHSO4+ 1.098e-012 1.017e-012 -11.959 -11.993 -0.033

Cl 5.728e-005

Cl- 5.728e-005 5.298e-005 -4.242 -4.276 -0.034

H(0) 2.821e-027

H2 1.410e-027 1.412e-027 -26.851 -26.850 0.001

K 3.326e-006

K+ 3.324e-006 3.074e-006 -5.478 -5.512 -0.034

KSO4- 1.671e-009 1.547e-009 -8.777 -8.810 -0.033

KOH 7.537e-013 7.546e-013 -12.123 -12.122 0.001

Mg 5.184e-004

Mg+2 4.947e-004 3.675e-004 -3.306 -3.435 -0.129

MgHCO3+ 1.396e-005 1.292e-005 -4.855 -4.889 -0.033

MgSO4 6.164e-006 6.171e-006 -5.210 -5.210 0.001

MgCO3 3.497e-006 3.502e-006 -5.456 -5.456 0.001

MgOH+ 1.023e-007 9.471e-008 -6.990 -7.024 -0.033

Na 1.001e-005

Na+ 9.986e-006 9.251e-006 -5.001 -5.034 -0.033

NaHCO3 1.561e-008 1.563e-008 -7.807 -7.806 0.001

NaSO4- 3.586e-009 3.320e-009 -8.445 -8.479 -0.033

NaCO3- 1.860e-009 1.722e-009 -8.730 -8.764 -0.033

NaOH 4.322e-012 4.327e-012 -11.364 -11.364 0.001

O(0) 3.251e-004

O2 1.625e-004 1.627e-004 -3.789 -3.789 0.001

S(6) 1.154e-004

SO4-2 9.694e-005 7.158e-005 -4.014 -4.145 -0.132

CaSO4 1.226e-005 1.228e-005 -4.911 -4.911 0.001

MgSO4 6.164e-006 6.171e-006 -5.210 -5.210 0.001

NaSO4- 3.586e-009 3.320e-009 -8.445 -8.479 -0.033

KSO4- 1.671e-009 1.547e-009 -8.777 -8.810 -0.033

HSO4- 1.063e-010 9.837e-011 -9.974 -10.007 -0.033

CaHSO4+ 1.098e-012 1.017e-012 -11.959 -11.993 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite 0.27 -8.07 -8.34 CaCO3

Calcite 0.41 -8.07 -8.48 CaCO3

CO2(g) -2.55 -4.02 -1.47 CO2

Dolomite 0.59 -16.50 -17.09 CaMg(CO3)2

Gypsum -2.63 -7.21 -4.58 CaSO4:2H2O

H2(g) -23.70 -26.85 -3.15 H2

H2O(g) -1.51 -0.00 1.51 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -0.90 -3.79 -2.89 O2

Initial solution 90. 30/8/2012 10:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.331e-003 3.331e-003

Ca 1.216e-003 1.216e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 3.926e-004 3.926e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.040

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 324

Density (g/cm3) = 0.99727

Activity of water = 1.000

Ionic strength = 5.169e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.343e-003

Total CO2 (mol/kg) = 3.343e-003

Temperature (deg C) = 25.030

Electrical balance (eq) = -1.369e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.01

Iterations = 7

Total H = 1.110157e+002

Total O = 5.551704e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.5509 0.7425

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.189e-006 1.100e-006 -5.925 -5.959 -0.034

H+ 9.777e-009 9.120e-009 -8.010 -8.040 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.343e-003

HCO3- 3.186e-003 2.957e-003 -2.497 -2.529 -0.032

CO2 6.054e-005 6.061e-005 -4.218 -4.217 0.001

CaHCO3+ 3.458e-005 3.209e-005 -4.461 -4.494 -0.032

CaCO3 2.172e-005 2.174e-005 -4.663 -4.663 0.001

CO3-2 2.052e-005 1.521e-005 -4.688 -4.818 -0.130

MgHCO3+ 1.370e-005 1.269e-005 -4.863 -4.897 -0.033

MgCO3 5.319e-006 5.325e-006 -5.274 -5.274 0.001

NaHCO3 1.537e-008 1.538e-008 -7.813 -7.813 0.001

NaCO3- 2.835e-009 2.625e-009 -8.547 -8.581 -0.033

Ca 1.216e-003

Ca+2 1.147e-003 8.503e-004 -2.940 -3.070 -0.130

CaHCO3+ 3.458e-005 3.209e-005 -4.461 -4.494 -0.032

CaCO3 2.172e-005 2.174e-005 -4.663 -4.663 0.001

CaSO4 1.216e-005 1.217e-005 -4.915 -4.915 0.001

CaOH+ 1.671e-008 1.547e-008 -7.777 -7.810 -0.033

CaHSO4+ 7.027e-013 6.507e-013 -12.153 -12.187 -0.033

Cl 5.728e-005

Cl- 5.728e-005 5.299e-005 -4.242 -4.276 -0.034

H(0) 1.176e-027

H2 5.880e-028 5.887e-028 -27.231 -27.230 0.001

K 3.326e-006

K+ 3.324e-006 3.075e-006 -5.478 -5.512 -0.034

KSO4- 1.675e-009 1.551e-009 -8.776 -8.809 -0.033

KOH 1.168e-012 1.169e-012 -11.933 -11.932 0.001

Mg 5.184e-004

Mg+2 4.931e-004 3.667e-004 -3.307 -3.436 -0.129

MgHCO3+ 1.370e-005 1.269e-005 -4.863 -4.897 -0.033

MgSO4 6.164e-006 6.171e-006 -5.210 -5.210 0.001

MgCO3 5.319e-006 5.325e-006 -5.274 -5.274 0.001

MgOH+ 1.581e-007 1.464e-007 -6.801 -6.835 -0.033

Na 1.001e-005

Na+ 9.985e-006 9.253e-006 -5.001 -5.034 -0.033

NaHCO3 1.537e-008 1.538e-008 -7.813 -7.813 0.001

NaSO4- 3.593e-009 3.328e-009 -8.445 -8.478 -0.033

NaCO3- 2.835e-009 2.625e-009 -8.547 -8.581 -0.033

NaOH 6.695e-012 6.703e-012 -11.174 -11.174 0.001

O(0) 3.926e-004

O2 1.963e-004 1.965e-004 -3.707 -3.707 0.001

S(6) 1.154e-004

SO4-2 9.704e-005 7.174e-005 -4.013 -4.144 -0.131

CaSO4 1.216e-005 1.217e-005 -4.915 -4.915 0.001

MgSO4 6.164e-006 6.171e-006 -5.210 -5.210 0.001

NaSO4- 3.593e-009 3.328e-009 -8.445 -8.478 -0.033

KSO4- 1.675e-009 1.551e-009 -8.776 -8.809 -0.033

HSO4- 6.874e-011 6.365e-011 -10.163 -10.196 -0.033

CaHSO4+ 7.027e-013 6.507e-013 -12.153 -12.187 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.21 -4.36 CaSO4

Aragonite 0.45 -7.89 -8.34 CaCO3

Calcite 0.59 -7.89 -8.48 CaCO3

CO2(g) -2.75 -4.22 -1.47 CO2

Dolomite 0.95 -16.14 -17.09 CaMg(CO3)2

Gypsum -2.63 -7.21 -4.58 CaSO4:2H2O

H2(g) -24.08 -27.23 -3.15 H2

H2O(g) -1.51 -0.00 1.51 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -0.81 -3.71 -2.89 O2

Initial solution 91. 30/8/2012 10:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.321e-003 3.321e-003

Ca 1.212e-003 1.212e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.376e-004 4.376e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.110

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 325

Density (g/cm3) = 0.99718

Activity of water = 1.000

Ionic strength = 5.147e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.314e-003

Total CO2 (mol/kg) = 3.314e-003

Temperature (deg C) = 25.360

Electrical balance (eq) = -1.342e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.98

Iterations = 7

Total H = 1.110156e+002

Total O = 5.551701e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.4654 0.7383

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.432e-006 1.325e-006 -5.844 -5.878 -0.034

H+ 8.321e-009 7.762e-009 -8.080 -8.110 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.314e-003

HCO3- 3.160e-003 2.932e-003 -2.500 -2.533 -0.032

CO2 5.090e-005 5.096e-005 -4.293 -4.293 0.001

CaHCO3+ 3.426e-005 3.180e-005 -4.465 -4.498 -0.032

CaCO3 2.549e-005 2.552e-005 -4.594 -4.593 0.001

CO3-2 2.406e-005 1.784e-005 -4.619 -4.749 -0.130

MgHCO3+ 1.359e-005 1.258e-005 -4.867 -4.900 -0.033

MgCO3 6.262e-006 6.269e-006 -5.203 -5.203 0.001

NaHCO3 1.524e-008 1.526e-008 -7.817 -7.816 0.001

NaCO3- 3.381e-009 3.131e-009 -8.471 -8.504 -0.033

Ca 1.212e-003

Ca+2 1.140e-003 8.453e-004 -2.943 -3.073 -0.130

CaHCO3+ 3.426e-005 3.180e-005 -4.465 -4.498 -0.032

CaCO3 2.549e-005 2.552e-005 -4.594 -4.593 0.001

CaSO4 1.213e-005 1.214e-005 -4.916 -4.916 0.001

CaOH+ 1.951e-008 1.807e-008 -7.710 -7.743 -0.033

CaHSO4+ 5.990e-013 5.547e-013 -12.223 -12.256 -0.033

Cl 5.728e-005

Cl- 5.728e-005 5.300e-005 -4.242 -4.276 -0.034

H(0) 8.491e-028

H2 4.246e-028 4.251e-028 -27.372 -27.372 0.001

K 3.326e-006

K+ 3.324e-006 3.076e-006 -5.478 -5.512 -0.034

KSO4- 1.685e-009 1.561e-009 -8.773 -8.807 -0.033

KOH 1.372e-012 1.374e-012 -11.863 -11.862 0.001

Mg 5.184e-004

Mg+2 4.922e-004 3.662e-004 -3.308 -3.436 -0.128

MgHCO3+ 1.359e-005 1.258e-005 -4.867 -4.900 -0.033

MgCO3 6.262e-006 6.269e-006 -5.203 -5.203 0.001

MgSO4 6.209e-006 6.217e-006 -5.207 -5.206 0.001

MgOH+ 1.910e-007 1.769e-007 -6.719 -6.752 -0.033

Na 1.001e-005

Na+ 9.985e-006 9.254e-006 -5.001 -5.034 -0.033

NaHCO3 1.524e-008 1.526e-008 -7.817 -7.816 0.001

NaSO4- 3.602e-009 3.336e-009 -8.443 -8.477 -0.033

NaCO3- 3.381e-009 3.131e-009 -8.471 -8.504 -0.033

NaOH 7.866e-012 7.876e-012 -11.104 -11.104 0.001

O(0) 4.376e-004

O2 2.188e-004 2.191e-004 -3.660 -3.659 0.001

S(6) 1.154e-004

SO4-2 9.703e-005 7.176e-005 -4.013 -4.144 -0.131

CaSO4 1.213e-005 1.214e-005 -4.916 -4.916 0.001

MgSO4 6.209e-006 6.217e-006 -5.207 -5.206 0.001

NaSO4- 3.602e-009 3.336e-009 -8.443 -8.477 -0.033

KSO4- 1.685e-009 1.561e-009 -8.773 -8.807 -0.033

HSO4- 5.894e-011 5.458e-011 -10.230 -10.263 -0.033

CaHSO4+ 5.990e-013 5.547e-013 -12.223 -12.256 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.85 -7.22 -4.36 CaSO4

Aragonite 0.52 -7.82 -8.34 CaCO3

Calcite 0.66 -7.82 -8.48 CaCO3

CO2(g) -2.82 -4.29 -1.47 CO2

Dolomite 1.09 -16.01 -17.10 CaMg(CO3)2

Gypsum -2.64 -7.22 -4.58 CaSO4:2H2O

H2(g) -24.22 -27.37 -3.15 H2

H2O(g) -1.50 -0.00 1.50 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -0.76 -3.66 -2.89 O2

Initial solution 92. 30/8/2012 10:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.310e-003 3.310e-003

Ca 1.208e-003 1.208e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.870e-004 4.870e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.260

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 324

Density (g/cm3) = 0.99713

Activity of water = 1.000

Ionic strength = 5.109e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.266e-003

Total CO2 (mol/kg) = 3.266e-003

Temperature (deg C) = 25.580

Electrical balance (eq) = -1.314e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.95

Iterations = 8

Total H = 1.110156e+002

Total O = 5.551693e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3088 0.7296

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.056e-006 1.903e-006 -5.687 -5.721 -0.034

H+ 5.890e-009 5.495e-009 -8.230 -8.260 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.266e-003

HCO3- 3.106e-003 2.883e-003 -2.508 -2.540 -0.032

CaCO3 3.536e-005 3.540e-005 -4.452 -4.451 0.001

CO2 3.533e-005 3.538e-005 -4.452 -4.451 0.001

CO3-2 3.353e-005 2.489e-005 -4.475 -4.604 -0.129

CaHCO3+ 3.344e-005 3.104e-005 -4.476 -4.508 -0.032

MgHCO3+ 1.332e-005 1.234e-005 -4.876 -4.909 -0.033

MgCO3 8.731e-006 8.741e-006 -5.059 -5.058 0.001

NaHCO3 1.499e-008 1.501e-008 -7.824 -7.824 0.001

NaCO3- 4.768e-009 4.417e-009 -8.322 -8.355 -0.033

Ca 1.208e-003

Ca+2 1.128e-003 8.366e-004 -2.948 -3.077 -0.130

CaCO3 3.536e-005 3.540e-005 -4.452 -4.451 0.001

CaHCO3+ 3.344e-005 3.104e-005 -4.476 -4.508 -0.032

CaSO4 1.205e-005 1.206e-005 -4.919 -4.919 0.001

CaOH+ 2.727e-008 2.526e-008 -7.564 -7.598 -0.033

CaHSO4+ 4.222e-013 3.911e-013 -12.374 -12.408 -0.033

Cl 5.728e-005

Cl- 5.728e-005 5.301e-005 -4.242 -4.276 -0.034

H(0) 4.246e-028

H2 2.123e-028 2.126e-028 -27.673 -27.673 0.001

K 3.326e-006

K+ 3.324e-006 3.076e-006 -5.478 -5.512 -0.034

KSO4- 1.694e-009 1.569e-009 -8.771 -8.804 -0.033

KOH 1.939e-012 1.941e-012 -11.713 -11.712 0.001

Mg 5.184e-004

Mg+2 4.899e-004 3.648e-004 -3.310 -3.438 -0.128

MgHCO3+ 1.332e-005 1.234e-005 -4.876 -4.909 -0.033

MgCO3 8.731e-006 8.741e-006 -5.059 -5.058 0.001

MgSO4 6.230e-006 6.237e-006 -5.206 -5.205 0.001

MgOH+ 2.741e-007 2.539e-007 -6.562 -6.595 -0.033

Na 1.001e-005

Na+ 9.984e-006 9.255e-006 -5.001 -5.034 -0.033

NaHCO3 1.499e-008 1.501e-008 -7.824 -7.824 0.001

NaCO3- 4.768e-009 4.417e-009 -8.322 -8.355 -0.033

NaSO4- 3.612e-009 3.346e-009 -8.442 -8.476 -0.033

NaOH 1.111e-011 1.113e-011 -10.954 -10.954 0.001

O(0) 4.870e-004

O2 2.435e-004 2.438e-004 -3.613 -3.613 0.001

S(6) 1.154e-004

SO4-2 9.709e-005 7.187e-005 -4.013 -4.143 -0.131

CaSO4 1.205e-005 1.206e-005 -4.919 -4.919 0.001

MgSO4 6.230e-006 6.237e-006 -5.206 -5.205 0.001

NaSO4- 3.612e-009 3.346e-009 -8.442 -8.476 -0.033

KSO4- 1.694e-009 1.569e-009 -8.771 -8.804 -0.033

HSO4- 4.198e-011 3.889e-011 -10.377 -10.410 -0.033

CaHSO4+ 4.222e-013 3.911e-013 -12.374 -12.408 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.86 -7.22 -4.36 CaSO4

Aragonite 0.66 -7.68 -8.34 CaCO3

Calcite 0.80 -7.68 -8.48 CaCO3

CO2(g) -2.98 -4.45 -1.47 CO2

Dolomite 1.38 -15.72 -17.10 CaMg(CO3)2

Gypsum -2.64 -7.22 -4.58 CaSO4:2H2O

H2(g) -24.52 -27.67 -3.15 H2

H2O(g) -1.50 -0.00 1.50 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -0.72 -3.61 -2.90 O2

Initial solution 93. 30/8/2012 10:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.310e-003 3.310e-003

Ca 1.208e-003 1.208e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.545e-004 5.545e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.370

pe = 4.000

Specific Conductance (uS/cm, 25 oC) = 325

Density (g/cm3) = 0.99704

Activity of water = 1.000

Ionic strength = 5.083e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.235e-003

Total CO2 (mol/kg) = 3.235e-003

Temperature (deg C) = 25.920

Electrical balance (eq) = -1.314e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.97

Iterations = 8

Total H = 1.110155e+002

Total O = 5.551691e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1849 0.7230

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.717e-006 2.515e-006 -5.566 -5.599 -0.034

H+ 4.571e-009 4.266e-009 -8.340 -8.370 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.235e-003

HCO3- 3.063e-003 2.843e-003 -2.514 -2.546 -0.032

CaCO3 4.519e-005 4.524e-005 -4.345 -4.344 0.001

CO3-2 4.286e-005 3.184e-005 -4.368 -4.497 -0.129

CaHCO3+ 3.289e-005 3.053e-005 -4.483 -4.515 -0.032

CO2 2.694e-005 2.697e-005 -4.570 -4.569 0.001

MgHCO3+ 1.310e-005 1.213e-005 -4.883 -4.916 -0.033

MgCO3 1.118e-005 1.119e-005 -4.952 -4.951 0.001

NaHCO3 1.478e-008 1.480e-008 -7.830 -7.830 0.001

NaCO3- 6.203e-009 5.747e-009 -8.207 -8.241 -0.033

Ca 1.208e-003

Ca+2 1.118e-003 8.302e-004 -2.951 -3.081 -0.129

CaCO3 4.519e-005 4.524e-005 -4.345 -4.344 0.001

CaHCO3+ 3.289e-005 3.053e-005 -4.483 -4.515 -0.032

CaSO4 1.200e-005 1.201e-005 -4.921 -4.920 0.001

CaOH+ 3.486e-008 3.230e-008 -7.458 -7.491 -0.033

CaHSO4+ 3.279e-013 3.038e-013 -12.484 -12.517 -0.033

Cl 5.728e-005

Cl- 5.728e-005 5.302e-005 -4.242 -4.276 -0.034

H(0) 2.550e-028

H2 1.275e-028 1.277e-028 -27.894 -27.894 0.001

K 3.326e-006

K+ 3.324e-006 3.077e-006 -5.478 -5.512 -0.034

KSO4- 1.705e-009 1.580e-009 -8.768 -8.801 -0.033

KOH 2.498e-012 2.501e-012 -11.602 -11.602 0.001

Mg 5.184e-004

Mg+2 4.875e-004 3.632e-004 -3.312 -3.440 -0.128

MgHCO3+ 1.310e-005 1.213e-005 -4.883 -4.916 -0.033

MgCO3 1.118e-005 1.119e-005 -4.952 -4.951 0.001

MgSO4 6.262e-006 6.269e-006 -5.203 -5.203 0.001

MgOH+ 3.624e-007 3.358e-007 -6.441 -6.474 -0.033

Na 1.001e-005

Na+ 9.983e-006 9.255e-006 -5.001 -5.034 -0.033

NaHCO3 1.478e-008 1.480e-008 -7.830 -7.830 0.001

NaCO3- 6.203e-009 5.747e-009 -8.207 -8.241 -0.033

NaSO4- 3.621e-009 3.355e-009 -8.441 -8.474 -0.033

NaOH 1.432e-011 1.433e-011 -10.844 -10.844 0.001

O(0) 5.545e-004

O2 2.773e-004 2.776e-004 -3.557 -3.557 0.001

S(6) 1.154e-004

SO4-2 9.710e-005 7.191e-005 -4.013 -4.143 -0.130

CaSO4 1.200e-005 1.201e-005 -4.921 -4.920 0.001

MgSO4 6.262e-006 6.269e-006 -5.203 -5.203 0.001

NaSO4- 3.621e-009 3.355e-009 -8.441 -8.474 -0.033

KSO4- 1.705e-009 1.580e-009 -8.768 -8.801 -0.033

HSO4- 3.285e-011 3.043e-011 -10.483 -10.517 -0.033

CaHSO4+ 3.279e-013 3.038e-013 -12.484 -12.517 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.86 -7.22 -4.36 CaSO4

Aragonite 0.76 -7.58 -8.34 CaCO3

Calcite 0.91 -7.58 -8.49 CaCO3

CO2(g) -3.09 -4.57 -1.48 CO2

Dolomite 1.60 -15.51 -17.11 CaMg(CO3)2

Gypsum -2.64 -7.22 -4.58 CaSO4:2H2O

H2(g) -24.74 -27.89 -3.15 H2

H2O(g) -1.49 -0.00 1.49 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -0.66 -3.56 -2.90 O2

Initial solution 94. 30/8/2012 11:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.310e-003 3.310e-003

Ca 1.208e-003 1.208e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.571e-004 6.571e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.370

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 328

Density (g/cm3) = 0.99694

Activity of water = 1.000

Ionic strength = 5.080e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.234e-003

Total CO2 (mol/kg) = 3.234e-003

Temperature (deg C) = 26.300

Electrical balance (eq) = -1.314e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.97

Iterations = 8

Total H = 1.110155e+002

Total O = 5.551701e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1721 0.7232

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.796e-006 2.587e-006 -5.554 -5.587 -0.034

H+ 4.571e-009 4.266e-009 -8.340 -8.370 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.234e-003

HCO3- 3.060e-003 2.841e-003 -2.514 -2.547 -0.032

CaCO3 4.582e-005 4.587e-005 -4.339 -4.338 0.001

CO3-2 4.315e-005 3.205e-005 -4.365 -4.494 -0.129

CaHCO3+ 3.302e-005 3.065e-005 -4.481 -4.514 -0.032

CO2 2.680e-005 2.683e-005 -4.572 -4.571 0.001

MgHCO3+ 1.310e-005 1.214e-005 -4.883 -4.916 -0.033

MgCO3 1.131e-005 1.133e-005 -4.946 -4.946 0.001

NaHCO3 1.477e-008 1.479e-008 -7.831 -7.830 0.001

NaCO3- 6.364e-009 5.896e-009 -8.196 -8.229 -0.033

Ca 1.208e-003

Ca+2 1.118e-003 8.295e-004 -2.952 -3.081 -0.129

CaCO3 4.582e-005 4.587e-005 -4.339 -4.338 0.001

CaHCO3+ 3.302e-005 3.065e-005 -4.481 -4.514 -0.032

CaSO4 1.202e-005 1.204e-005 -4.920 -4.919 0.001

CaOH+ 3.483e-008 3.227e-008 -7.458 -7.491 -0.033

CaHSO4+ 3.301e-013 3.058e-013 -12.481 -12.515 -0.033

Cl 5.728e-005

Cl- 5.728e-005 5.302e-005 -4.242 -4.276 -0.034

H(0) 2.541e-028

H2 1.270e-028 1.272e-028 -27.896 -27.896 0.001

K 3.326e-006

K+ 3.324e-006 3.077e-006 -5.478 -5.512 -0.034

KSO4- 1.715e-009 1.589e-009 -8.766 -8.799 -0.033

KOH 2.498e-012 2.501e-012 -11.602 -11.602 0.001

Mg 5.184e-004

Mg+2 4.873e-004 3.630e-004 -3.312 -3.440 -0.128

MgHCO3+ 1.310e-005 1.214e-005 -4.883 -4.916 -0.033

MgCO3 1.131e-005 1.133e-005 -4.946 -4.946 0.001

MgSO4 6.314e-006 6.321e-006 -5.200 -5.199 0.001

MgOH+ 3.748e-007 3.472e-007 -6.426 -6.459 -0.033

Na 1.001e-005

Na+ 9.983e-006 9.255e-006 -5.001 -5.034 -0.033

NaHCO3 1.477e-008 1.479e-008 -7.831 -7.830 0.001

NaCO3- 6.364e-009 5.896e-009 -8.196 -8.229 -0.033

NaSO4- 3.627e-009 3.360e-009 -8.440 -8.474 -0.033

NaOH 1.432e-011 1.433e-011 -10.844 -10.844 0.001

O(0) 6.571e-004

O2 3.285e-004 3.289e-004 -3.483 -3.483 0.001

S(6) 1.154e-004

SO4-2 9.703e-005 7.185e-005 -4.013 -4.144 -0.130

CaSO4 1.202e-005 1.204e-005 -4.920 -4.919 0.001

MgSO4 6.314e-006 6.321e-006 -5.200 -5.199 0.001

NaSO4- 3.627e-009 3.360e-009 -8.440 -8.474 -0.033

KSO4- 1.715e-009 1.589e-009 -8.766 -8.799 -0.033

HSO4- 3.310e-011 3.066e-011 -10.480 -10.513 -0.033

CaHSO4+ 3.301e-013 3.058e-013 -12.481 -12.515 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.86 -7.22 -4.37 CaSO4

Aragonite 0.77 -7.58 -8.34 CaCO3

Calcite 0.91 -7.58 -8.49 CaCO3

CO2(g) -3.09 -4.57 -1.48 CO2

Dolomite 1.61 -15.51 -17.12 CaMg(CO3)2

Gypsum -2.64 -7.22 -4.58 CaSO4:2H2O

H2(g) -24.74 -27.90 -3.16 H2

H2O(g) -1.48 -0.00 1.48 H2O

Halite -10.89 -9.31 1.58 NaCl

O2(g) -0.58 -3.48 -2.90 O2

Initial solution 95. 30/8/2012 11:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.310e-003 3.310e-003

Ca 1.208e-003 1.208e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 7.077e-004 7.077e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.640

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 326

Density (g/cm3) = 0.99679

Activity of water = 1.000

Ionic strength = 4.990e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.140e-003

Total CO2 (mol/kg) = 3.140e-003

Temperature (deg C) = 26.840

Electrical balance (eq) = -1.314e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.02

Iterations = 8

Total H = 1.110154e+002

Total O = 5.551680e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8659 0.7063

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 5.416e-006 5.015e-006 -5.266 -5.300 -0.033

H+ 2.454e-009 2.291e-009 -8.610 -8.640 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.140e-003

HCO3- 2.906e-003 2.699e-003 -2.537 -2.569 -0.032

CaCO3 8.061e-005 8.070e-005 -4.094 -4.093 0.000

CO3-2 7.697e-005 5.729e-005 -4.114 -4.242 -0.128

CaHCO3+ 3.074e-005 2.856e-005 -4.512 -4.544 -0.032

MgCO3 2.008e-005 2.011e-005 -4.697 -4.697 0.000

CO2 1.359e-005 1.360e-005 -4.867 -4.866 0.000

MgHCO3+ 1.228e-005 1.139e-005 -4.911 -4.944 -0.033

NaHCO3 1.403e-008 1.405e-008 -7.853 -7.852 0.000

NaCO3- 1.168e-008 1.083e-008 -7.933 -7.965 -0.033

Ca 1.208e-003

Ca+2 1.085e-003 8.072e-004 -2.964 -3.093 -0.129

CaCO3 8.061e-005 8.070e-005 -4.094 -4.093 0.000

CaHCO3+ 3.074e-005 2.856e-005 -4.512 -4.544 -0.032

CaSO4 1.181e-005 1.182e-005 -4.928 -4.927 0.000

CaOH+ 6.308e-008 5.847e-008 -7.200 -7.233 -0.033

CaHSO4+ 1.752e-013 1.624e-013 -12.756 -12.789 -0.033

Cl 5.728e-005

Cl- 5.728e-005 5.305e-005 -4.242 -4.275 -0.033

H(0) 7.288e-029

H2 3.644e-029 3.648e-029 -28.438 -28.438 0.000

K 3.326e-006

K+ 3.324e-006 3.078e-006 -5.478 -5.512 -0.033

KSO4- 1.738e-009 1.611e-009 -8.760 -8.793 -0.033

KOH 4.654e-012 4.659e-012 -11.332 -11.332 0.000

Mg 5.184e-004

Mg+2 4.790e-004 3.575e-004 -3.320 -3.447 -0.127

MgCO3 2.008e-005 2.011e-005 -4.697 -4.697 0.000

MgHCO3+ 1.228e-005 1.139e-005 -4.911 -4.944 -0.033

MgSO4 6.332e-006 6.339e-006 -5.198 -5.198 0.000

MgOH+ 7.210e-007 6.683e-007 -6.142 -6.175 -0.033

Na 1.001e-005

Na+ 9.978e-006 9.255e-006 -5.001 -5.034 -0.033

NaHCO3 1.403e-008 1.405e-008 -7.853 -7.852 0.000

NaCO3- 1.168e-008 1.083e-008 -7.933 -7.965 -0.033

NaSO4- 3.653e-009 3.386e-009 -8.437 -8.470 -0.033

NaOH 2.666e-011 2.669e-011 -10.574 -10.574 0.000

O(0) 7.077e-004

O2 3.539e-004 3.543e-004 -3.451 -3.451 0.000

S(6) 1.154e-004

SO4-2 9.723e-005 7.215e-005 -4.012 -4.142 -0.130

CaSO4 1.181e-005 1.182e-005 -4.928 -4.927 0.000

MgSO4 6.332e-006 6.339e-006 -5.198 -5.198 0.000

NaSO4- 3.653e-009 3.386e-009 -8.437 -8.470 -0.033

KSO4- 1.738e-009 1.611e-009 -8.760 -8.793 -0.033

HSO4- 1.805e-011 1.673e-011 -10.743 -10.776 -0.033

CaHSO4+ 1.752e-013 1.624e-013 -12.756 -12.789 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.87 -7.23 -4.37 CaSO4

Aragonite 1.01 -7.33 -8.35 CaCO3

Calcite 1.16 -7.33 -8.49 CaCO3

CO2(g) -3.38 -4.87 -1.49 CO2

Dolomite 2.11 -15.02 -17.13 CaMg(CO3)2

Gypsum -2.65 -7.23 -4.58 CaSO4:2H2O

H2(g) -25.28 -28.44 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.55 -3.45 -2.91 O2

Initial solution 96. 30/8/2012 11:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.300e-003 3.300e-003

Ca 1.205e-003 1.205e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 8.227e-004 8.227e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.860

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 321

Density (g/cm3) = 0.99665

Activity of water = 1.000

Ionic strength = 4.870e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.024e-003

Total CO2 (mol/kg) = 3.024e-003

Temperature (deg C) = 27.320

Electrical balance (eq) = -1.284e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.04

Iterations = 7

Total H = 1.110152e+002

Total O = 5.551658e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.6230 0.6929

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.306e-006 8.624e-006 -5.031 -5.064 -0.033

H+ 1.478e-009 1.380e-009 -8.830 -8.860 -0.030

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.024e-003

HCO3- 2.704e-003 2.513e-003 -2.568 -2.600 -0.032

CaCO3 1.224e-004 1.226e-004 -3.912 -3.912 0.000

CO3-2 1.197e-004 8.935e-005 -3.922 -4.049 -0.127

MgCO3 3.096e-005 3.100e-005 -4.509 -4.509 0.000

CaHCO3+ 2.776e-005 2.580e-005 -4.557 -4.588 -0.032

MgHCO3+ 1.124e-005 1.043e-005 -4.949 -4.982 -0.033

CO2 7.584e-006 7.593e-006 -5.120 -5.120 0.000

NaCO3- 1.865e-008 1.730e-008 -7.729 -7.762 -0.033

NaHCO3 1.307e-008 1.308e-008 -7.884 -7.883 0.000

Ca 1.205e-003

Ca+2 1.043e-003 7.780e-004 -2.982 -3.109 -0.127

CaCO3 1.224e-004 1.226e-004 -3.912 -3.912 0.000

CaHCO3+ 2.776e-005 2.580e-005 -4.557 -4.588 -0.032

CaSO4 1.150e-005 1.151e-005 -4.939 -4.939 0.000

CaOH+ 1.008e-007 9.353e-008 -6.996 -7.029 -0.033

CaHSO4+ 1.034e-013 9.592e-014 -12.986 -13.018 -0.033

Cl 5.728e-005

Cl- 5.728e-005 5.309e-005 -4.242 -4.275 -0.033

H(0) 2.634e-029

H2 1.317e-029 1.318e-029 -28.880 -28.880 0.000

K 3.326e-006

K+ 3.324e-006 3.081e-006 -5.478 -5.511 -0.033

KSO4- 1.764e-009 1.636e-009 -8.754 -8.786 -0.033

KOH 7.730e-012 7.738e-012 -11.112 -11.111 0.000

Mg 5.184e-004

Mg+2 4.687e-004 3.508e-004 -3.329 -3.455 -0.126

MgCO3 3.096e-005 3.100e-005 -4.509 -4.509 0.000

MgHCO3+ 1.124e-005 1.043e-005 -4.949 -4.982 -0.033

MgSO4 6.328e-006 6.335e-006 -5.199 -5.198 0.000

MgOH+ 1.224e-006 1.136e-006 -5.912 -5.945 -0.033

Na 1.001e-005

Na+ 9.972e-006 9.257e-006 -5.001 -5.034 -0.032

NaCO3- 1.865e-008 1.730e-008 -7.729 -7.762 -0.033

NaHCO3 1.307e-008 1.308e-008 -7.884 -7.883 0.000

NaSO4- 3.684e-009 3.418e-009 -8.434 -8.466 -0.033

NaOH 4.425e-011 4.430e-011 -10.354 -10.354 0.000

O(0) 8.227e-004

O2 4.114e-004 4.118e-004 -3.386 -3.385 0.000

S(6) 1.154e-004

SO4-2 9.754e-005 7.260e-005 -4.011 -4.139 -0.128

CaSO4 1.150e-005 1.151e-005 -4.939 -4.939 0.000

MgSO4 6.328e-006 6.335e-006 -5.199 -5.198 0.000

NaSO4- 3.684e-009 3.418e-009 -8.434 -8.466 -0.033

KSO4- 1.764e-009 1.636e-009 -8.754 -8.786 -0.033

HSO4- 1.105e-011 1.025e-011 -10.956 -10.989 -0.033

CaHSO4+ 1.034e-013 9.592e-014 -12.986 -13.018 -0.033

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 1.19 -7.16 -8.35 CaCO3

Calcite 1.34 -7.16 -8.49 CaCO3

CO2(g) -3.62 -5.12 -1.49 CO2

Dolomite 2.48 -14.66 -17.14 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -25.72 -28.88 -3.16 H2

H2O(g) -1.45 -0.00 1.45 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.48 -3.39 -2.91 O2

Initial solution 97. 30/8/2012 11:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.279e-003 3.279e-003

Ca 1.197e-003 1.197e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.434e-004 9.434e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.960

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 319

Density (g/cm3) = 0.99653

Activity of water = 1.000

Ionic strength = 4.785e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.944e-003

Total CO2 (mol/kg) = 2.944e-003

Temperature (deg C) = 27.780

Electrical balance (eq) = -1.229e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.00

Iterations = 7

Total H = 1.110151e+002

Total O = 5.551646e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.5004 0.6867

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.211e-005 1.123e-005 -4.917 -4.950 -0.033

H+ 1.173e-009 1.096e-009 -8.931 -8.960 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.944e-003

HCO3- 2.574e-003 2.394e-003 -2.589 -2.621 -0.032

CaCO3 1.458e-004 1.459e-004 -3.836 -3.836 0.000

CO3-2 1.445e-004 1.081e-004 -3.840 -3.966 -0.126

MgCO3 3.730e-005 3.734e-005 -4.428 -4.428 0.000

CaHCO3+ 2.591e-005 2.410e-005 -4.587 -4.618 -0.032

MgHCO3+ 1.061e-005 9.846e-006 -4.974 -5.007 -0.032

CO2 5.709e-006 5.715e-006 -5.243 -5.243 0.000

NaCO3- 2.306e-008 2.141e-008 -7.637 -7.669 -0.032

NaHCO3 1.245e-008 1.246e-008 -7.905 -7.904 0.000

Ca 1.197e-003

Ca+2 1.014e-003 7.581e-004 -2.994 -3.120 -0.126

CaCO3 1.458e-004 1.459e-004 -3.836 -3.836 0.000

CaHCO3+ 2.591e-005 2.410e-005 -4.587 -4.618 -0.032

CaSO4 1.130e-005 1.131e-005 -4.947 -4.946 0.000

CaOH+ 1.236e-007 1.147e-007 -6.908 -6.940 -0.032

CaHSO4+ 8.112e-014 7.529e-014 -13.091 -13.123 -0.032

Cl 5.728e-005

Cl- 5.728e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 1.654e-029

H2 8.272e-030 8.281e-030 -29.082 -29.082 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.784e-009 1.656e-009 -8.748 -8.781 -0.032

KOH 9.736e-012 9.747e-012 -11.012 -11.011 0.000

Mg 5.184e-004

Mg+2 4.626e-004 3.470e-004 -3.335 -3.460 -0.125

MgCO3 3.730e-005 3.734e-005 -4.428 -4.428 0.000

MgHCO3+ 1.061e-005 9.846e-006 -4.974 -5.007 -0.032

MgSO4 6.356e-006 6.363e-006 -5.197 -5.196 0.000

MgOH+ 1.587e-006 1.473e-006 -5.799 -5.832 -0.032

Na 1.001e-005

Na+ 9.968e-006 9.258e-006 -5.001 -5.033 -0.032

NaCO3- 2.306e-008 2.141e-008 -7.637 -7.669 -0.032

NaHCO3 1.245e-008 1.246e-008 -7.905 -7.904 0.000

NaSO4- 3.708e-009 3.441e-009 -8.431 -8.463 -0.032

NaOH 5.572e-011 5.578e-011 -10.254 -10.254 0.000

O(0) 9.434e-004

O2 4.717e-004 4.722e-004 -3.326 -3.326 0.000

S(6) 1.154e-004

SO4-2 9.771e-005 7.288e-005 -4.010 -4.137 -0.127

CaSO4 1.130e-005 1.131e-005 -4.947 -4.946 0.000

MgSO4 6.356e-006 6.363e-006 -5.197 -5.196 0.000

NaSO4- 3.708e-009 3.441e-009 -8.431 -8.463 -0.032

KSO4- 1.784e-009 1.656e-009 -8.748 -8.781 -0.032

HSO4- 8.900e-012 8.261e-012 -11.051 -11.083 -0.032

CaHSO4+ 8.112e-014 7.529e-014 -13.091 -13.123 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.37 CaSO4

Aragonite 1.27 -7.09 -8.35 CaCO3

Calcite 1.41 -7.09 -8.50 CaCO3

CO2(g) -3.74 -5.24 -1.50 CO2

Dolomite 2.64 -14.51 -17.15 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -25.92 -29.08 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.41 -3.33 -2.91 O2

Initial solution 98. 30/8/2012 12:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.269e-003 3.269e-003

Ca 1.193e-003 1.193e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 9.803e-004 9.803e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.980

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 320

Density (g/cm3) = 0.99638

Activity of water = 1.000

Ionic strength = 4.755e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.918e-003

Total CO2 (mol/kg) = 2.918e-003

Temperature (deg C) = 28.300

Electrical balance (eq) = -1.199e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.97

Iterations = 7

Total H = 1.110150e+002

Total O = 5.551642e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.4423 0.6844

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.317e-005 1.222e-005 -4.880 -4.913 -0.033

H+ 1.120e-009 1.047e-009 -8.951 -8.980 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.918e-003

HCO3- 2.535e-003 2.358e-003 -2.596 -2.628 -0.031

CaCO3 1.522e-004 1.523e-004 -3.818 -3.817 0.000

CO3-2 1.504e-004 1.125e-004 -3.823 -3.949 -0.126

MgCO3 3.902e-005 3.907e-005 -4.409 -4.408 0.000

CaHCO3+ 2.546e-005 2.368e-005 -4.594 -4.626 -0.031

MgHCO3+ 1.044e-005 9.692e-006 -4.981 -5.014 -0.032

CO2 5.341e-006 5.346e-006 -5.272 -5.272 0.000

NaCO3- 2.464e-008 2.287e-008 -7.608 -7.641 -0.032

NaHCO3 1.226e-008 1.227e-008 -7.911 -7.911 0.000

Ca 1.193e-003

Ca+2 1.004e-003 7.513e-004 -2.998 -3.124 -0.126

CaCO3 1.522e-004 1.523e-004 -3.818 -3.817 0.000

CaHCO3+ 2.546e-005 2.368e-005 -4.594 -4.626 -0.031

CaSO4 1.126e-005 1.127e-005 -4.949 -4.948 0.000

CaOH+ 1.283e-007 1.191e-007 -6.892 -6.924 -0.032

CaHSO4+ 7.769e-014 7.212e-014 -13.110 -13.142 -0.032

Cl 5.728e-005

Cl- 5.728e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 1.501e-029

H2 7.506e-030 7.514e-030 -29.125 -29.124 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.801e-009 1.672e-009 -8.744 -8.777 -0.032

KOH 1.020e-011 1.021e-011 -10.992 -10.991 0.000

Mg 5.184e-004

Mg+2 4.608e-004 3.458e-004 -3.336 -3.461 -0.125

MgCO3 3.902e-005 3.907e-005 -4.409 -4.408 0.000

MgHCO3+ 1.044e-005 9.692e-006 -4.981 -5.014 -0.032

MgSO4 6.422e-006 6.429e-006 -5.192 -5.192 0.000

MgOH+ 1.734e-006 1.610e-006 -5.761 -5.793 -0.032

Na 1.001e-005

Na+ 9.967e-006 9.258e-006 -5.001 -5.033 -0.032

NaCO3- 2.464e-008 2.287e-008 -7.608 -7.641 -0.032

NaHCO3 1.226e-008 1.227e-008 -7.911 -7.911 0.000

NaSO4- 3.720e-009 3.454e-009 -8.429 -8.462 -0.032

NaOH 5.835e-011 5.841e-011 -10.234 -10.234 0.000

O(0) 9.803e-004

O2 4.901e-004 4.907e-004 -3.310 -3.309 0.000

S(6) 1.154e-004

SO4-2 9.769e-005 7.291e-005 -4.010 -4.137 -0.127

CaSO4 1.126e-005 1.127e-005 -4.949 -4.948 0.000

MgSO4 6.422e-006 6.429e-006 -5.192 -5.192 0.000

NaSO4- 3.720e-009 3.454e-009 -8.429 -8.462 -0.032

KSO4- 1.801e-009 1.672e-009 -8.744 -8.777 -0.032

HSO4- 8.601e-012 7.984e-012 -11.065 -11.098 -0.032

CaHSO4+ 7.769e-014 7.212e-014 -13.110 -13.142 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.26 -4.38 CaSO4

Aragonite 1.28 -7.07 -8.36 CaCO3

Calcite 1.43 -7.07 -8.50 CaCO3

CO2(g) -3.77 -5.27 -1.51 CO2

Dolomite 2.68 -14.48 -17.17 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -25.96 -29.12 -3.16 H2

H2O(g) -1.43 -0.00 1.43 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.39 -3.31 -2.92 O2

Initial solution 99. 30/8/2012 12:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.228e-003 3.228e-003

Ca 1.178e-003 1.178e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.077e-003 1.077e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.090

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 316

Density (g/cm3) = 0.99625

Activity of water = 1.000

Ionic strength = 4.637e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.804e-003

Total CO2 (mol/kg) = 2.804e-003

Temperature (deg C) = 28.730

Electrical balance (eq) = -1.085e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.85

Iterations = 7

Total H = 1.110148e+002

Total O = 5.551618e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.3078 0.6773

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.750e-005 1.624e-005 -4.757 -4.789 -0.032

H+ 8.691e-010 8.128e-010 -9.061 -9.090 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.804e-003

HCO3- 2.360e-003 2.197e-003 -2.627 -2.658 -0.031

CO3-2 1.814e-004 1.362e-004 -3.741 -3.866 -0.125

CaCO3 1.792e-004 1.794e-004 -3.747 -3.746 0.000

MgCO3 4.688e-005 4.693e-005 -4.329 -4.329 0.000

CaHCO3+ 2.298e-005 2.139e-005 -4.639 -4.670 -0.031

MgHCO3+ 9.609e-006 8.927e-006 -5.017 -5.049 -0.032

CO2 3.846e-006 3.850e-006 -5.415 -5.415 0.000

NaCO3- 3.043e-008 2.827e-008 -7.517 -7.549 -0.032

NaHCO3 1.143e-008 1.144e-008 -7.942 -7.942 0.000

Ca 1.178e-003

Ca+2 9.652e-004 7.241e-004 -3.015 -3.140 -0.125

CaCO3 1.792e-004 1.794e-004 -3.747 -3.746 0.000

CaHCO3+ 2.298e-005 2.139e-005 -4.639 -4.670 -0.031

CaSO4 1.096e-005 1.097e-005 -4.960 -4.960 0.000

CaOH+ 1.591e-007 1.478e-007 -6.798 -6.830 -0.032

CaHSO4+ 5.899e-014 5.480e-014 -13.229 -13.261 -0.032

Cl 5.728e-005

Cl- 5.728e-005 5.317e-005 -4.242 -4.274 -0.032

H(0) 9.008e-030

H2 4.504e-030 4.509e-030 -29.346 -29.346 0.000

K 3.326e-006

K+ 3.324e-006 3.086e-006 -5.478 -5.511 -0.032

KSO4- 1.825e-009 1.696e-009 -8.739 -8.771 -0.032

KOH 1.315e-011 1.316e-011 -10.881 -10.881 0.000

Mg 5.184e-004

Mg+2 4.532e-004 3.411e-004 -3.344 -3.467 -0.123

MgCO3 4.688e-005 4.693e-005 -4.329 -4.329 0.000

MgHCO3+ 9.609e-006 8.927e-006 -5.017 -5.049 -0.032

MgSO4 6.441e-006 6.448e-006 -5.191 -5.191 0.000

MgOH+ 2.287e-006 2.125e-006 -5.641 -5.673 -0.032

Na 1.001e-005

Na+ 9.962e-006 9.261e-006 -5.002 -5.033 -0.032

NaCO3- 3.043e-008 2.827e-008 -7.517 -7.549 -0.032

NaHCO3 1.143e-008 1.144e-008 -7.942 -7.942 0.000

NaSO4- 3.751e-009 3.484e-009 -8.426 -8.458 -0.032

NaOH 7.519e-011 7.527e-011 -10.124 -10.123 0.000

O(0) 1.077e-003

O2 5.386e-004 5.392e-004 -3.269 -3.268 0.000

S(6) 1.154e-004

SO4-2 9.797e-005 7.334e-005 -4.009 -4.135 -0.126

CaSO4 1.096e-005 1.097e-005 -4.960 -4.960 0.000

MgSO4 6.441e-006 6.448e-006 -5.191 -5.191 0.000

NaSO4- 3.751e-009 3.484e-009 -8.426 -8.458 -0.032

KSO4- 1.825e-009 1.696e-009 -8.739 -8.771 -0.032

HSO4- 6.776e-012 6.295e-012 -11.169 -11.201 -0.032

CaHSO4+ 5.899e-014 5.480e-014 -13.229 -13.261 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.90 -7.27 -4.38 CaSO4

Aragonite 1.35 -7.01 -8.36 CaCO3

Calcite 1.50 -7.01 -8.50 CaCO3

CO2(g) -3.90 -5.41 -1.51 CO2

Dolomite 2.84 -14.34 -17.18 CaMg(CO3)2

Gypsum -2.69 -7.27 -4.58 CaSO4:2H2O

H2(g) -26.18 -29.35 -3.17 H2

H2O(g) -1.41 -0.00 1.41 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.35 -3.27 -2.92 O2

Initial solution 100. 30/8/2012 12:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.228e-003 3.228e-003

Ca 1.178e-003 1.178e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.200e-003 1.200e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.080

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 319

Density (g/cm3) = 0.99608

Activity of water = 1.000

Ionic strength = 4.634e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.806e-003

Total CO2 (mol/kg) = 2.806e-003

Temperature (deg C) = 29.320

Electrical balance (eq) = -1.085e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.85

Iterations = 7

Total H = 1.110148e+002

Total O = 5.551631e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.2819 0.6771

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.785e-005 1.657e-005 -4.748 -4.781 -0.032

H+ 8.893e-010 8.318e-010 -9.051 -9.080 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.806e-003

HCO3- 2.363e-003 2.200e-003 -2.627 -2.658 -0.031

CaCO3 1.794e-004 1.796e-004 -3.746 -3.746 0.000

CO3-2 1.794e-004 1.346e-004 -3.746 -3.871 -0.125

MgCO3 4.677e-005 4.682e-005 -4.330 -4.330 0.000

CaHCO3+ 2.317e-005 2.156e-005 -4.635 -4.666 -0.031

MgHCO3+ 9.648e-006 8.963e-006 -5.016 -5.048 -0.032

CO2 3.917e-006 3.921e-006 -5.407 -5.407 0.000

NaCO3- 3.098e-008 2.878e-008 -7.509 -7.541 -0.032

NaHCO3 1.144e-008 1.145e-008 -7.942 -7.941 0.000

Ca 1.178e-003

Ca+2 9.647e-004 7.236e-004 -3.016 -3.140 -0.125

CaCO3 1.794e-004 1.796e-004 -3.746 -3.746 0.000

CaHCO3+ 2.317e-005 2.156e-005 -4.635 -4.666 -0.031

CaSO4 1.099e-005 1.100e-005 -4.959 -4.958 0.000

CaOH+ 1.554e-007 1.444e-007 -6.809 -6.841 -0.032

CaHSO4+ 6.105e-014 5.671e-014 -13.214 -13.246 -0.032

Cl 5.728e-005

Cl- 5.728e-005 5.317e-005 -4.242 -4.274 -0.032

H(0) 9.379e-030

H2 4.689e-030 4.694e-030 -29.329 -29.328 0.000

K 3.326e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.841e-009 1.710e-009 -8.735 -8.767 -0.032

KOH 1.285e-011 1.286e-011 -10.891 -10.891 0.000

Mg 5.184e-004

Mg+2 4.531e-004 3.410e-004 -3.344 -3.467 -0.123

MgCO3 4.677e-005 4.682e-005 -4.330 -4.330 0.000

MgHCO3+ 9.648e-006 8.963e-006 -5.016 -5.048 -0.032

MgSO4 6.526e-006 6.533e-006 -5.185 -5.185 0.000

MgOH+ 2.353e-006 2.186e-006 -5.628 -5.660 -0.032

Na 1.001e-005

Na+ 9.961e-006 9.260e-006 -5.002 -5.033 -0.032

NaCO3- 3.098e-008 2.878e-008 -7.509 -7.541 -0.032

NaHCO3 1.144e-008 1.145e-008 -7.942 -7.941 0.000

NaSO4- 3.759e-009 3.492e-009 -8.425 -8.457 -0.032

NaOH 7.347e-011 7.355e-011 -10.134 -10.133 0.000

O(0) 1.200e-003

O2 6.002e-004 6.008e-004 -3.222 -3.221 0.000

S(6) 1.154e-004

SO4-2 9.785e-005 7.324e-005 -4.009 -4.135 -0.126

CaSO4 1.099e-005 1.100e-005 -4.959 -4.958 0.000

MgSO4 6.526e-006 6.533e-006 -5.185 -5.185 0.000

NaSO4- 3.759e-009 3.492e-009 -8.425 -8.457 -0.032

KSO4- 1.841e-009 1.710e-009 -8.735 -8.767 -0.032

HSO4- 7.017e-012 6.518e-012 -11.154 -11.186 -0.032

CaHSO4+ 6.105e-014 5.671e-014 -13.214 -13.246 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.28 -4.38 CaSO4

Aragonite 1.35 -7.01 -8.36 CaCO3

Calcite 1.49 -7.01 -8.51 CaCO3

CO2(g) -3.89 -5.41 -1.52 CO2

Dolomite 2.84 -14.35 -17.19 CaMg(CO3)2

Gypsum -2.69 -7.28 -4.58 CaSO4:2H2O

H2(g) -26.16 -29.33 -3.17 H2

H2O(g) -1.40 -0.00 1.40 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.30 -3.22 -2.92 O2

Initial solution 101. 30/8/2012 12:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.186e-003 3.186e-003

Ca 1.164e-003 1.164e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.187e-003 1.187e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.050

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 321

Density (g/cm3) = 0.99595

Activity of water = 1.000

Ionic strength = 4.608e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.788e-003

Total CO2 (mol/kg) = 2.788e-003

Temperature (deg C) = 29.750

Electrical balance (eq) = -9.732e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.66

Iterations = 7

Total H = 1.110149e+002

Total O = 5.551624e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.2761 0.6777

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.718e-005 1.595e-005 -4.765 -4.797 -0.032

H+ 9.528e-010 8.913e-010 -9.021 -9.050 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.788e-003

HCO3- 2.367e-003 2.203e-003 -2.626 -2.657 -0.031

CaCO3 1.699e-004 1.700e-004 -3.770 -3.769 0.000

CO3-2 1.689e-004 1.269e-004 -3.772 -3.897 -0.124

MgCO3 4.458e-005 4.462e-005 -4.351 -4.350 0.000

CaHCO3+ 2.321e-005 2.161e-005 -4.634 -4.665 -0.031

MgHCO3+ 9.735e-006 9.045e-006 -5.012 -5.044 -0.032

CO2 4.187e-006 4.191e-006 -5.378 -5.378 0.000

NaCO3- 2.981e-008 2.770e-008 -7.526 -7.558 -0.032

NaHCO3 1.146e-008 1.148e-008 -7.941 -7.940 0.000

Ca 1.164e-003

Ca+2 9.593e-004 7.199e-004 -3.018 -3.143 -0.125

CaCO3 1.699e-004 1.700e-004 -3.770 -3.769 0.000

CaHCO3+ 2.321e-005 2.161e-005 -4.634 -4.665 -0.031

CaSO4 1.097e-005 1.099e-005 -4.960 -4.959 0.000

CaOH+ 1.443e-007 1.340e-007 -6.841 -6.873 -0.032

CaHSO4+ 6.568e-014 6.103e-014 -13.183 -13.214 -0.032

Cl 5.728e-005

Cl- 5.728e-005 5.317e-005 -4.242 -4.274 -0.032

H(0) 1.072e-029

H2 5.362e-030 5.368e-030 -29.271 -29.270 0.000

K 3.326e-006

K+ 3.324e-006 3.086e-006 -5.478 -5.511 -0.032

KSO4- 1.854e-009 1.722e-009 -8.732 -8.764 -0.032

KOH 1.199e-011 1.200e-011 -10.921 -10.921 0.000

Mg 5.184e-004

Mg+2 4.552e-004 3.427e-004 -3.342 -3.465 -0.123

MgCO3 4.458e-005 4.462e-005 -4.351 -4.350 0.000

MgHCO3+ 9.735e-006 9.045e-006 -5.012 -5.044 -0.032

MgSO4 6.627e-006 6.634e-006 -5.179 -5.178 0.000

MgOH+ 2.292e-006 2.129e-006 -5.640 -5.672 -0.032

Na 1.001e-005

Na+ 9.962e-006 9.262e-006 -5.002 -5.033 -0.032

NaCO3- 2.981e-008 2.770e-008 -7.526 -7.558 -0.032

NaHCO3 1.146e-008 1.148e-008 -7.941 -7.940 0.000

NaSO4- 3.768e-009 3.501e-009 -8.424 -8.456 -0.032

NaOH 6.858e-011 6.865e-011 -10.164 -10.163 0.000

O(0) 1.187e-003

O2 5.933e-004 5.939e-004 -3.227 -3.226 0.000

S(6) 1.154e-004

SO4-2 9.777e-005 7.321e-005 -4.010 -4.135 -0.126

CaSO4 1.097e-005 1.099e-005 -4.960 -4.959 0.000

MgSO4 6.627e-006 6.634e-006 -5.179 -5.178 0.000

NaSO4- 3.768e-009 3.501e-009 -8.424 -8.456 -0.032

KSO4- 1.854e-009 1.722e-009 -8.732 -8.764 -0.032

HSO4- 7.588e-012 7.050e-012 -11.120 -11.152 -0.032

CaHSO4+ 6.568e-014 6.103e-014 -13.183 -13.214 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.28 -4.38 CaSO4

Aragonite 1.33 -7.04 -8.37 CaCO3

Calcite 1.47 -7.04 -8.51 CaCO3

CO2(g) -3.86 -5.38 -1.52 CO2

Dolomite 2.80 -14.40 -17.20 CaMg(CO3)2

Gypsum -2.69 -7.28 -4.58 CaSO4:2H2O

H2(g) -26.10 -29.27 -3.17 H2

H2O(g) -1.39 -0.00 1.39 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.30 -3.23 -2.92 O2

Initial solution 102. 30/8/2012 13:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.135e-003 3.135e-003

Ca 1.145e-003 1.145e-003

Cl 5.728e-005 5.728e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.252e-003 1.252e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.040

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 320

Density (g/cm3) = 0.99583

Activity of water = 1.000

Ionic strength = 4.559e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.747e-003

Total CO2 (mol/kg) = 2.747e-003

Temperature (deg C) = 30.140

Electrical balance (eq) = -8.296e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.43

Iterations = 7

Total H = 1.110148e+002

Total O = 5.551619e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.2606 0.6776

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.726e-005 1.603e-005 -4.763 -4.795 -0.032

H+ 9.748e-010 9.120e-010 -9.011 -9.040 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.747e-003

HCO3- 2.338e-003 2.177e-003 -2.631 -2.662 -0.031

CaCO3 1.646e-004 1.648e-004 -3.784 -3.783 0.000

CO3-2 1.640e-004 1.233e-004 -3.785 -3.909 -0.124

MgCO3 4.372e-005 4.377e-005 -4.359 -4.359 0.000

CaHCO3+ 2.275e-005 2.119e-005 -4.643 -4.674 -0.031

MgHCO3+ 9.663e-006 8.981e-006 -5.015 -5.047 -0.032

CO2 4.217e-006 4.221e-006 -5.375 -5.375 0.000

NaCO3- 2.954e-008 2.745e-008 -7.530 -7.561 -0.032

NaHCO3 1.133e-008 1.134e-008 -7.946 -7.945 0.000

Ca 1.145e-003

Ca+2 9.464e-004 7.111e-004 -3.024 -3.148 -0.124

CaCO3 1.646e-004 1.648e-004 -3.784 -3.783 0.000

CaHCO3+ 2.275e-005 2.119e-005 -4.643 -4.674 -0.031

CaSO4 1.089e-005 1.090e-005 -4.963 -4.963 0.000

CaOH+ 1.392e-007 1.294e-007 -6.856 -6.888 -0.032

CaHSO4+ 6.703e-014 6.230e-014 -13.174 -13.206 -0.032

Cl 5.728e-005

Cl- 5.728e-005 5.319e-005 -4.242 -4.274 -0.032

H(0) 1.119e-029

H2 5.594e-030 5.600e-030 -29.252 -29.252 0.000

K 3.326e-006

K+ 3.324e-006 3.087e-006 -5.478 -5.511 -0.032

KSO4- 1.868e-009 1.736e-009 -8.729 -8.760 -0.032

KOH 1.172e-011 1.173e-011 -10.931 -10.931 0.000

Mg 5.184e-004

Mg+2 4.560e-004 3.437e-004 -3.341 -3.464 -0.123

MgCO3 4.372e-005 4.377e-005 -4.359 -4.359 0.000

MgHCO3+ 9.663e-006 8.981e-006 -5.015 -5.047 -0.032

MgSO4 6.719e-006 6.726e-006 -5.173 -5.172 0.000

MgOH+ 2.323e-006 2.159e-006 -5.634 -5.666 -0.032

Na 1.001e-005

Na+ 9.963e-006 9.265e-006 -5.002 -5.033 -0.032

NaCO3- 2.954e-008 2.745e-008 -7.530 -7.561 -0.032

NaHCO3 1.133e-008 1.134e-008 -7.946 -7.945 0.000

NaSO4- 3.781e-009 3.514e-009 -8.422 -8.454 -0.032

NaOH 6.704e-011 6.711e-011 -10.174 -10.173 0.000

O(0) 1.252e-003

O2 6.258e-004 6.265e-004 -3.204 -3.203 0.000

S(6) 1.154e-004

SO4-2 9.776e-005 7.329e-005 -4.010 -4.135 -0.125

CaSO4 1.089e-005 1.090e-005 -4.963 -4.963 0.000

MgSO4 6.719e-006 6.726e-006 -5.173 -5.172 0.000

NaSO4- 3.781e-009 3.514e-009 -8.422 -8.454 -0.032

KSO4- 1.868e-009 1.736e-009 -8.729 -8.760 -0.032

HSO4- 7.840e-012 7.287e-012 -11.106 -11.137 -0.032

CaHSO4+ 6.703e-014 6.230e-014 -13.174 -13.206 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.90 -7.28 -4.39 CaSO4

Aragonite 1.31 -7.06 -8.37 CaCO3

Calcite 1.45 -7.06 -8.51 CaCO3

CO2(g) -3.85 -5.37 -1.53 CO2

Dolomite 2.78 -14.43 -17.21 CaMg(CO3)2

Gypsum -2.70 -7.28 -4.58 CaSO4:2H2O

H2(g) -26.08 -29.25 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.28 -3.20 -2.93 O2

Initial solution 103. 30/8/2012 13:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.073e-003 3.073e-003

Ca 1.122e-003 1.122e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.248e-003 1.248e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.040

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 318

Density (g/cm3) = 0.99572

Activity of water = 1.000

Ionic strength = 4.494e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.691e-003

Total CO2 (mol/kg) = 2.691e-003

Temperature (deg C) = 30.490

Electrical balance (eq) = -6.592e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.16

Iterations = 7

Total H = 1.110148e+002

Total O = 5.551602e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.2324 0.6767

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.769e-005 1.643e-005 -4.752 -4.784 -0.032

H+ 9.745e-010 9.120e-010 -9.011 -9.040 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.691e-003

HCO3- 2.290e-003 2.133e-003 -2.640 -2.671 -0.031

CO3-2 1.614e-004 1.216e-004 -3.792 -3.915 -0.123

CaCO3 1.608e-004 1.609e-004 -3.794 -3.793 0.000

MgCO3 4.343e-005 4.347e-005 -4.362 -4.362 0.000

CaHCO3+ 2.199e-005 2.049e-005 -4.658 -4.689 -0.031

MgHCO3+ 9.503e-006 8.836e-006 -5.022 -5.054 -0.032

CO2 4.118e-006 4.122e-006 -5.385 -5.385 0.000

NaCO3- 2.962e-008 2.754e-008 -7.528 -7.560 -0.032

NaHCO3 1.111e-008 1.112e-008 -7.954 -7.954 0.000

Ca 1.122e-003

Ca+2 9.287e-004 6.989e-004 -3.032 -3.156 -0.123

CaCO3 1.608e-004 1.609e-004 -3.794 -3.793 0.000

CaHCO3+ 2.199e-005 2.049e-005 -4.658 -4.689 -0.031

CaSO4 1.076e-005 1.077e-005 -4.968 -4.968 0.000

CaOH+ 1.368e-007 1.272e-007 -6.864 -6.896 -0.032

CaHSO4+ 6.652e-014 6.185e-014 -13.177 -13.209 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.321e-005 -4.242 -4.274 -0.032

H(0) 1.115e-029

H2 5.575e-030 5.581e-030 -29.254 -29.253 0.000

K 3.326e-006

K+ 3.324e-006 3.088e-006 -5.478 -5.510 -0.032

KSO4- 1.883e-009 1.751e-009 -8.725 -8.757 -0.032

KOH 1.173e-011 1.174e-011 -10.931 -10.930 0.000

Mg 5.184e-004

Mg+2 4.563e-004 3.445e-004 -3.341 -3.463 -0.122

MgCO3 4.343e-005 4.347e-005 -4.362 -4.362 0.000

MgHCO3+ 9.503e-006 8.836e-006 -5.022 -5.054 -0.032

MgSO4 6.807e-006 6.814e-006 -5.167 -5.167 0.000

MgOH+ 2.400e-006 2.231e-006 -5.620 -5.651 -0.032

Na 1.001e-005

Na+ 9.963e-006 9.269e-006 -5.002 -5.033 -0.031

NaCO3- 2.962e-008 2.754e-008 -7.528 -7.560 -0.032

NaHCO3 1.111e-008 1.112e-008 -7.954 -7.954 0.000

NaSO4- 3.797e-009 3.531e-009 -8.421 -8.452 -0.032

NaOH 6.707e-011 6.714e-011 -10.173 -10.173 0.000

O(0) 1.248e-003

O2 6.242e-004 6.249e-004 -3.205 -3.204 0.000

S(6) 1.154e-004

SO4-2 9.780e-005 7.345e-005 -4.010 -4.134 -0.124

CaSO4 1.076e-005 1.077e-005 -4.968 -4.968 0.000

MgSO4 6.807e-006 6.814e-006 -5.167 -5.167 0.000

NaSO4- 3.797e-009 3.531e-009 -8.421 -8.452 -0.032

KSO4- 1.883e-009 1.751e-009 -8.725 -8.757 -0.032

HSO4- 7.916e-012 7.360e-012 -11.101 -11.133 -0.032

CaHSO4+ 6.652e-014 6.185e-014 -13.177 -13.209 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.90 -7.29 -4.39 CaSO4

Aragonite 1.30 -7.07 -8.37 CaCO3

Calcite 1.44 -7.07 -8.51 CaCO3

CO2(g) -3.86 -5.38 -1.53 CO2

Dolomite 2.77 -14.45 -17.22 CaMg(CO3)2

Gypsum -2.71 -7.29 -4.58 CaSO4:2H2O

H2(g) -26.08 -29.25 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.27 -3.20 -2.93 O2

Initial solution 104. 30/8/2012 13:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.021e-003 3.021e-003

Ca 1.104e-003 1.104e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.410e-003 1.410e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.050

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 314

Density (g/cm3) = 0.99568

Activity of water = 1.000

Ionic strength = 4.437e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.639e-003

Total CO2 (mol/kg) = 2.639e-003

Temperature (deg C) = 30.610

Electrical balance (eq) = -5.188e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.92

Iterations = 7

Total H = 1.110147e+002

Total O = 5.551602e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.2260 0.6766

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.825e-005 1.696e-005 -4.739 -4.771 -0.032

H+ 9.519e-010 8.913e-010 -9.021 -9.050 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.639e-003

HCO3- 2.240e-003 2.088e-003 -2.650 -2.680 -0.031

CO3-2 1.618e-004 1.220e-004 -3.791 -3.914 -0.123

CaCO3 1.592e-004 1.594e-004 -3.798 -3.797 0.000

MgCO3 4.372e-005 4.376e-005 -4.359 -4.359 0.000

CaHCO3+ 2.121e-005 1.976e-005 -4.674 -4.704 -0.031

MgHCO3+ 9.314e-006 8.663e-006 -5.031 -5.062 -0.031

CO2 3.935e-006 3.939e-006 -5.405 -5.405 0.000

NaCO3- 2.990e-008 2.781e-008 -7.524 -7.556 -0.031

NaHCO3 1.087e-008 1.089e-008 -7.964 -7.963 0.000

Ca 1.104e-003

Ca+2 9.124e-004 6.877e-004 -3.040 -3.163 -0.123

CaCO3 1.592e-004 1.594e-004 -3.798 -3.797 0.000

CaHCO3+ 2.121e-005 1.976e-005 -4.674 -4.704 -0.031

CaSO4 1.063e-005 1.064e-005 -4.974 -4.973 0.000

CaOH+ 1.377e-007 1.280e-007 -6.861 -6.893 -0.031

CaHSO4+ 6.427e-014 5.978e-014 -13.192 -13.223 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.324e-005 -4.242 -4.274 -0.032

H(0) 1.064e-029

H2 5.318e-030 5.323e-030 -29.274 -29.274 0.000

K 3.326e-006

K+ 3.324e-006 3.089e-006 -5.478 -5.510 -0.032

KSO4- 1.892e-009 1.759e-009 -8.723 -8.755 -0.031

KOH 1.201e-011 1.202e-011 -10.921 -10.920 0.000

Mg 5.184e-004

Mg+2 4.560e-004 3.448e-004 -3.341 -3.462 -0.121

MgCO3 4.372e-005 4.376e-005 -4.359 -4.359 0.000

MgHCO3+ 9.314e-006 8.663e-006 -5.031 -5.062 -0.031

MgSO4 6.852e-006 6.859e-006 -5.164 -5.164 0.000

MgOH+ 2.483e-006 2.309e-006 -5.605 -5.636 -0.031

Na 1.001e-005

Na+ 9.963e-006 9.273e-006 -5.002 -5.033 -0.031

NaCO3- 2.990e-008 2.781e-008 -7.524 -7.556 -0.031

NaHCO3 1.087e-008 1.089e-008 -7.964 -7.963 0.000

NaSO4- 3.809e-009 3.543e-009 -8.419 -8.451 -0.031

NaOH 6.866e-011 6.873e-011 -10.163 -10.163 0.000

O(0) 1.410e-003

O2 7.052e-004 7.059e-004 -3.152 -3.151 0.000

S(6) 1.154e-004

SO4-2 9.789e-005 7.363e-005 -4.009 -4.133 -0.124

CaSO4 1.063e-005 1.064e-005 -4.974 -4.973 0.000

MgSO4 6.852e-006 6.859e-006 -5.164 -5.164 0.000

NaSO4- 3.809e-009 3.543e-009 -8.419 -8.451 -0.031

KSO4- 1.892e-009 1.759e-009 -8.723 -8.755 -0.031

HSO4- 7.773e-012 7.231e-012 -11.109 -11.141 -0.031

CaHSO4+ 6.427e-014 5.978e-014 -13.192 -13.223 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.91 -7.30 -4.39 CaSO4

Aragonite 1.30 -7.08 -8.37 CaCO3

Calcite 1.44 -7.08 -8.51 CaCO3

CO2(g) -3.87 -5.40 -1.53 CO2

Dolomite 2.77 -14.45 -17.22 CaMg(CO3)2

Gypsum -2.71 -7.30 -4.58 CaSO4:2H2O

H2(g) -26.10 -29.27 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.22 -3.15 -2.93 O2

Initial solution 105. 30/8/2012 13:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.969e-003 2.969e-003

Ca 1.085e-003 1.085e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.410e-003 1.410e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.080

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 310

Density (g/cm3) = 0.99565

Activity of water = 1.000

Ionic strength = 4.369e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.575e-003

Total CO2 (mol/kg) = 2.575e-003

Temperature (deg C) = 30.680

Electrical balance (eq) = -3.751e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.68

Iterations = 7

Total H = 1.110147e+002

Total O = 5.551583e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.1905 0.6746

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.964e-005 1.826e-005 -4.707 -4.738 -0.032

H+ 8.880e-010 8.318e-010 -9.052 -9.080 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.575e-003

HCO3- 2.167e-003 2.021e-003 -2.664 -2.695 -0.030

CO3-2 1.677e-004 1.267e-004 -3.776 -3.897 -0.122

CaCO3 1.622e-004 1.624e-004 -3.790 -3.789 0.000

MgCO3 4.537e-005 4.542e-005 -4.343 -4.343 0.000

CaHCO3+ 2.011e-005 1.875e-005 -4.697 -4.727 -0.030

MgHCO3+ 8.999e-006 8.375e-006 -5.046 -5.077 -0.031

CO2 3.552e-006 3.555e-006 -5.450 -5.449 0.000

NaCO3- 3.115e-008 2.899e-008 -7.507 -7.538 -0.031

NaHCO3 1.053e-008 1.054e-008 -7.978 -7.977 0.000

Ca 1.085e-003

Ca+2 8.919e-004 6.736e-004 -3.050 -3.172 -0.122

CaCO3 1.622e-004 1.624e-004 -3.790 -3.789 0.000

CaHCO3+ 2.011e-005 1.875e-005 -4.697 -4.727 -0.030

CaSO4 1.045e-005 1.046e-005 -4.981 -4.980 0.000

CaOH+ 1.444e-007 1.344e-007 -6.840 -6.872 -0.031

CaHSO4+ 5.902e-014 5.493e-014 -13.229 -13.260 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.326e-005 -4.242 -4.274 -0.032

H(0) 9.257e-030

H2 4.629e-030 4.633e-030 -29.335 -29.334 0.000

K 3.326e-006

K+ 3.324e-006 3.091e-006 -5.478 -5.510 -0.032

KSO4- 1.900e-009 1.769e-009 -8.721 -8.752 -0.031

KOH 1.287e-011 1.288e-011 -10.890 -10.890 0.000

Mg 5.184e-004

Mg+2 4.545e-004 3.443e-004 -3.342 -3.463 -0.121

MgCO3 4.537e-005 4.542e-005 -4.343 -4.343 0.000

MgHCO3+ 8.999e-006 8.375e-006 -5.046 -5.077 -0.031

MgSO4 6.877e-006 6.884e-006 -5.163 -5.162 0.000

MgOH+ 2.671e-006 2.486e-006 -5.573 -5.605 -0.031

Na 1.001e-005

Na+ 9.962e-006 9.276e-006 -5.002 -5.033 -0.031

NaCO3- 3.115e-008 2.899e-008 -7.507 -7.538 -0.031

NaHCO3 1.053e-008 1.054e-008 -7.978 -7.977 0.000

NaSO4- 3.824e-009 3.559e-009 -8.417 -8.449 -0.031

NaOH 7.360e-011 7.368e-011 -10.133 -10.133 0.000

O(0) 1.410e-003

O2 7.052e-004 7.059e-004 -3.152 -3.151 0.000

S(6) 1.154e-004

SO4-2 9.804e-005 7.389e-005 -4.009 -4.131 -0.123

CaSO4 1.045e-005 1.046e-005 -4.981 -4.980 0.000

MgSO4 6.877e-006 6.884e-006 -5.163 -5.162 0.000

NaSO4- 3.824e-009 3.559e-009 -8.417 -8.449 -0.031

KSO4- 1.900e-009 1.769e-009 -8.721 -8.752 -0.031

HSO4- 7.288e-012 6.782e-012 -11.137 -11.169 -0.031

CaHSO4+ 5.902e-014 5.493e-014 -13.229 -13.260 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.91 -7.30 -4.39 CaSO4

Aragonite 1.31 -7.07 -8.37 CaCO3

Calcite 1.45 -7.07 -8.51 CaCO3

CO2(g) -3.92 -5.45 -1.53 CO2

Dolomite 2.79 -14.43 -17.22 CaMg(CO3)2

Gypsum -2.72 -7.30 -4.58 CaSO4:2H2O

H2(g) -26.16 -29.33 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.22 -3.15 -2.93 O2

Initial solution 106. 30/8/2012 14:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.949e-003 2.949e-003

Ca 1.077e-003 1.077e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.469e-003 1.469e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.080

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 310

Density (g/cm3) = 0.99557

Activity of water = 1.000

Ionic strength = 4.345e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.555e-003

Total CO2 (mol/kg) = 2.555e-003

Temperature (deg C) = 30.950

Electrical balance (eq) = -3.183e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.58

Iterations = 7

Total H = 1.110146e+002

Total O = 5.551583e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.1733 0.6742

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.002e-005 1.862e-005 -4.699 -4.730 -0.032

H+ 8.879e-010 8.318e-010 -9.052 -9.080 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.555e-003

HCO3- 2.149e-003 2.004e-003 -2.668 -2.698 -0.030

CO3-2 1.670e-004 1.262e-004 -3.777 -3.899 -0.121

CaCO3 1.616e-004 1.617e-004 -3.792 -3.791 0.000

MgCO3 4.541e-005 4.546e-005 -4.343 -4.342 0.000

CaHCO3+ 1.987e-005 1.853e-005 -4.702 -4.732 -0.030

MgHCO3+ 8.940e-006 8.321e-006 -5.049 -5.080 -0.031

CO2 3.514e-006 3.517e-006 -5.454 -5.454 0.000

NaCO3- 3.144e-008 2.927e-008 -7.502 -7.534 -0.031

NaHCO3 1.044e-008 1.045e-008 -7.981 -7.981 0.000

Ca 1.077e-003

Ca+2 8.854e-004 6.690e-004 -3.053 -3.175 -0.122

CaCO3 1.616e-004 1.617e-004 -3.792 -3.791 0.000

CaHCO3+ 1.987e-005 1.853e-005 -4.702 -4.732 -0.030

CaSO4 1.041e-005 1.042e-005 -4.983 -4.982 0.000

CaOH+ 1.434e-007 1.335e-007 -6.843 -6.875 -0.031

CaHSO4+ 5.900e-014 5.491e-014 -13.229 -13.260 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.327e-005 -4.242 -4.274 -0.031

H(0) 9.234e-030

H2 4.617e-030 4.621e-030 -29.336 -29.335 0.000

K 3.326e-006

K+ 3.324e-006 3.091e-006 -5.478 -5.510 -0.031

KSO4- 1.910e-009 1.778e-009 -8.719 -8.750 -0.031

KOH 1.287e-011 1.289e-011 -10.890 -10.890 0.000

Mg 5.184e-004

Mg+2 4.544e-004 3.444e-004 -3.343 -3.463 -0.120

MgCO3 4.541e-005 4.546e-005 -4.343 -4.342 0.000

MgHCO3+ 8.940e-006 8.321e-006 -5.049 -5.080 -0.031

MgSO4 6.929e-006 6.936e-006 -5.159 -5.159 0.000

MgOH+ 2.735e-006 2.546e-006 -5.563 -5.594 -0.031

Na 1.001e-005

Na+ 9.961e-006 9.277e-006 -5.002 -5.033 -0.031

NaCO3- 3.144e-008 2.927e-008 -7.502 -7.534 -0.031

NaHCO3 1.044e-008 1.045e-008 -7.981 -7.981 0.000

NaSO4- 3.832e-009 3.567e-009 -8.417 -8.448 -0.031

NaOH 7.361e-011 7.369e-011 -10.133 -10.133 0.000

O(0) 1.469e-003

O2 7.343e-004 7.350e-004 -3.134 -3.134 0.000

S(6) 1.154e-004

SO4-2 9.803e-005 7.392e-005 -4.009 -4.131 -0.123

CaSO4 1.041e-005 1.042e-005 -4.983 -4.982 0.000

MgSO4 6.929e-006 6.936e-006 -5.159 -5.159 0.000

NaSO4- 3.832e-009 3.567e-009 -8.417 -8.448 -0.031

KSO4- 1.910e-009 1.778e-009 -8.719 -8.750 -0.031

HSO4- 7.335e-012 6.827e-012 -11.135 -11.166 -0.031

CaHSO4+ 5.900e-014 5.491e-014 -13.229 -13.260 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.91 -7.31 -4.39 CaSO4

Aragonite 1.30 -7.07 -8.38 CaCO3

Calcite 1.44 -7.07 -8.52 CaCO3

CO2(g) -3.92 -5.45 -1.53 CO2

Dolomite 2.79 -14.44 -17.23 CaMg(CO3)2

Gypsum -2.72 -7.31 -4.58 CaSO4:2H2O

H2(g) -26.16 -29.34 -3.18 H2

H2O(g) -1.36 -0.00 1.36 H2O

Halite -10.90 -9.31 1.60 NaCl

O2(g) -0.20 -3.13 -2.93 O2

Initial solution 107. 30/8/2012 14:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.938e-003 2.938e-003

Ca 1.074e-003 1.074e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.320e-003 1.320e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.080

pe = 4.000

Specific Conductance (uS/cm, 31 oC) = 311

Density (g/cm3) = 0.99550

Activity of water = 1.000

Ionic strength = 4.332e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.545e-003

Total CO2 (mol/kg) = 2.545e-003

Temperature (deg C) = 31.180

Electrical balance (eq) = -2.899e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.53

Iterations = 7

Total H = 1.110146e+002

Total O = 5.551565e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.1434 0.6729

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.035e-005 1.893e-005 -4.691 -4.723 -0.031

H+ 8.879e-010 8.318e-010 -9.052 -9.080 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.545e-003

HCO3- 2.138e-003 1.994e-003 -2.670 -2.700 -0.030

CO3-2 1.668e-004 1.261e-004 -3.778 -3.899 -0.121

CaCO3 1.617e-004 1.618e-004 -3.791 -3.791 0.000

MgCO3 4.552e-005 4.557e-005 -4.342 -4.341 0.000

CaHCO3+ 1.975e-005 1.842e-005 -4.704 -4.735 -0.030

MgHCO3+ 8.907e-006 8.291e-006 -5.050 -5.081 -0.031

CO2 3.490e-006 3.493e-006 -5.457 -5.457 0.000

NaCO3- 3.177e-008 2.957e-008 -7.498 -7.529 -0.031

NaHCO3 1.039e-008 1.040e-008 -7.983 -7.983 0.000

Ca 1.074e-003

Ca+2 8.817e-004 6.664e-004 -3.055 -3.176 -0.122

CaCO3 1.617e-004 1.618e-004 -3.791 -3.791 0.000

CaHCO3+ 1.975e-005 1.842e-005 -4.704 -4.735 -0.030

CaSO4 1.039e-005 1.040e-005 -4.983 -4.983 0.000

CaOH+ 1.428e-007 1.330e-007 -6.845 -6.876 -0.031

CaHSO4+ 5.908e-014 5.499e-014 -13.229 -13.260 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.328e-005 -4.242 -4.273 -0.031

H(0) 9.213e-030

H2 4.607e-030 4.611e-030 -29.337 -29.336 0.000

K 3.326e-006

K+ 3.324e-006 3.092e-006 -5.478 -5.510 -0.031

KSO4- 1.917e-009 1.785e-009 -8.717 -8.748 -0.031

KOH 1.287e-011 1.289e-011 -10.890 -10.890 0.000

Mg 5.184e-004

Mg+2 4.542e-004 3.444e-004 -3.343 -3.463 -0.120

MgCO3 4.552e-005 4.557e-005 -4.342 -4.341 0.000

MgHCO3+ 8.907e-006 8.291e-006 -5.050 -5.081 -0.031

MgSO4 6.968e-006 6.975e-006 -5.157 -5.156 0.000

MgOH+ 2.790e-006 2.597e-006 -5.554 -5.586 -0.031

Na 1.001e-005

Na+ 9.961e-006 9.278e-006 -5.002 -5.033 -0.031

NaCO3- 3.177e-008 2.957e-008 -7.498 -7.529 -0.031

NaHCO3 1.039e-008 1.040e-008 -7.983 -7.983 0.000

NaSO4- 3.837e-009 3.572e-009 -8.416 -8.447 -0.031

NaOH 7.362e-011 7.369e-011 -10.133 -10.133 0.000

O(0) 1.320e-003

O2 6.599e-004 6.605e-004 -3.181 -3.180 0.000

S(6) 1.154e-004

SO4-2 9.801e-005 7.392e-005 -4.009 -4.131 -0.122

CaSO4 1.039e-005 1.040e-005 -4.983 -4.983 0.000

MgSO4 6.968e-006 6.975e-006 -5.157 -5.156 0.000

NaSO4- 3.837e-009 3.572e-009 -8.416 -8.447 -0.031

KSO4- 1.917e-009 1.785e-009 -8.717 -8.748 -0.031

HSO4- 7.374e-012 6.864e-012 -11.132 -11.163 -0.031

CaHSO4+ 5.908e-014 5.499e-014 -13.229 -13.260 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.91 -7.31 -4.39 CaSO4

Aragonite 1.30 -7.08 -8.38 CaCO3

Calcite 1.44 -7.08 -8.52 CaCO3

CO2(g) -3.92 -5.46 -1.54 CO2

Dolomite 2.79 -14.44 -17.23 CaMg(CO3)2

Gypsum -2.72 -7.31 -4.58 CaSO4:2H2O

H2(g) -26.16 -29.34 -3.18 H2

H2O(g) -1.35 -0.00 1.35 H2O

Halite -10.90 -9.31 1.60 NaCl

O2(g) -0.25 -3.18 -2.93 O2

Initial solution 108. 30/8/2012 14:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.897e-003 2.897e-003

Ca 1.059e-003 1.059e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.319e-003 1.319e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.120

pe = 4.000

Specific Conductance (uS/cm, 31 oC) = 308

Density (g/cm3) = 0.99543

Activity of water = 1.000

Ionic strength = 4.265e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.481e-003

Total CO2 (mol/kg) = 2.481e-003

Temperature (deg C) = 31.400

Electrical balance (eq) = -1.779e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.33

Iterations = 7

Total H = 1.110145e+002

Total O = 5.551546e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.0859 0.6699

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.265e-005 2.108e-005 -4.645 -4.676 -0.031

H+ 8.094e-010 7.586e-010 -9.092 -9.120 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.481e-003

HCO3- 2.058e-003 1.920e-003 -2.687 -2.717 -0.030

CO3-2 1.764e-004 1.336e-004 -3.754 -3.874 -0.121

CaCO3 1.685e-004 1.687e-004 -3.773 -3.773 0.000

MgCO3 4.820e-005 4.825e-005 -4.317 -4.317 0.000

CaHCO3+ 1.864e-005 1.739e-005 -4.730 -4.760 -0.030

MgHCO3+ 8.547e-006 7.959e-006 -5.068 -5.099 -0.031

CO2 3.058e-006 3.061e-006 -5.515 -5.514 0.000

NaCO3- 3.401e-008 3.167e-008 -7.468 -7.499 -0.031

NaHCO3 1.001e-008 1.002e-008 -8.000 -7.999 0.000

Ca 1.059e-003

Ca+2 8.611e-004 6.521e-004 -3.065 -3.186 -0.121

CaCO3 1.685e-004 1.687e-004 -3.773 -3.773 0.000

CaHCO3+ 1.864e-005 1.739e-005 -4.730 -4.760 -0.030

CaSO4 1.022e-005 1.023e-005 -4.991 -4.990 0.000

CaOH+ 1.532e-007 1.426e-007 -6.815 -6.846 -0.031

CaHSO4+ 5.313e-014 4.948e-014 -13.275 -13.306 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.330e-005 -4.242 -4.273 -0.031

H(0) 7.647e-030

H2 3.824e-030 3.827e-030 -29.418 -29.417 0.000

K 3.326e-006

K+ 3.324e-006 3.093e-006 -5.478 -5.510 -0.031

KSO4- 1.931e-009 1.798e-009 -8.714 -8.745 -0.031

KOH 1.412e-011 1.414e-011 -10.850 -10.850 0.000

Mg 5.184e-004

Mg+2 4.515e-004 3.430e-004 -3.345 -3.465 -0.119

MgCO3 4.820e-005 4.825e-005 -4.317 -4.317 0.000

MgHCO3+ 8.547e-006 7.959e-006 -5.068 -5.099 -0.031

MgSO4 7.000e-006 7.007e-006 -5.155 -5.154 0.000

MgOH+ 3.103e-006 2.890e-006 -5.508 -5.539 -0.031

Na 1.001e-005

Na+ 9.959e-006 9.280e-006 -5.002 -5.032 -0.031

NaCO3- 3.401e-008 3.167e-008 -7.468 -7.499 -0.031

NaHCO3 1.001e-008 1.002e-008 -8.000 -7.999 0.000

NaSO4- 3.854e-009 3.589e-009 -8.414 -8.445 -0.031

NaOH 8.074e-011 8.082e-011 -10.093 -10.092 0.000

O(0) 1.319e-003

O2 6.596e-004 6.602e-004 -3.181 -3.180 0.000

S(6) 1.154e-004

SO4-2 9.814e-005 7.417e-005 -4.008 -4.130 -0.122

CaSO4 1.022e-005 1.023e-005 -4.991 -4.990 0.000

MgSO4 7.000e-006 7.007e-006 -5.155 -5.154 0.000

NaSO4- 3.854e-009 3.589e-009 -8.414 -8.445 -0.031

KSO4- 1.931e-009 1.798e-009 -8.714 -8.745 -0.031

HSO4- 6.778e-012 6.312e-012 -11.169 -11.200 -0.031

CaHSO4+ 5.313e-014 4.948e-014 -13.275 -13.306 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.92 -7.32 -4.39 CaSO4

Aragonite 1.32 -7.06 -8.38 CaCO3

Calcite 1.46 -7.06 -8.52 CaCO3

CO2(g) -3.97 -5.51 -1.54 CO2

Dolomite 2.84 -14.40 -17.24 CaMg(CO3)2

Gypsum -2.73 -7.32 -4.59 CaSO4:2H2O

H2(g) -26.24 -29.42 -3.18 H2

H2O(g) -1.35 -0.00 1.35 H2O

Halite -10.90 -9.31 1.60 NaCl

O2(g) -0.24 -3.18 -2.94 O2

Initial solution 109. 30/8/2012 15:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.845e-003 2.845e-003

Ca 1.040e-003 1.040e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.353e-003 1.353e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.160

pe = 4.000

Specific Conductance (uS/cm, 31 oC) = 303

Density (g/cm3) = 0.99538

Activity of water = 1.000

Ionic strength = 4.191e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.410e-003

Total CO2 (mol/kg) = 2.410e-003

Temperature (deg C) = 31.520

Electrical balance (eq) = -3.427e-006

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.07

Iterations = 7

Total H = 1.110145e+002

Total O = 5.551529e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.0391 0.6673

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.503e-005 2.331e-005 -4.601 -4.632 -0.031

H+ 7.379e-010 6.918e-010 -9.132 -9.160 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.410e-003

HCO3- 1.972e-003 1.840e-003 -2.705 -2.735 -0.030

CO3-2 1.854e-004 1.407e-004 -3.732 -3.852 -0.120

CaCO3 1.737e-004 1.739e-004 -3.760 -3.760 0.000

MgCO3 5.069e-005 5.074e-005 -4.295 -4.295 0.000

CaHCO3+ 1.745e-005 1.629e-005 -4.758 -4.788 -0.030

MgHCO3+ 8.166e-006 7.609e-006 -5.088 -5.119 -0.031

CO2 2.671e-006 2.673e-006 -5.573 -5.573 0.000

NaCO3- 3.602e-008 3.357e-008 -7.443 -7.474 -0.031

NaHCO3 9.599e-009 9.608e-009 -8.018 -8.017 0.000

Ca 1.040e-003

Ca+2 8.386e-004 6.363e-004 -3.076 -3.196 -0.120

CaCO3 1.737e-004 1.739e-004 -3.760 -3.760 0.000

CaHCO3+ 1.745e-005 1.629e-005 -4.758 -4.788 -0.030

CaSO4 1.002e-005 1.003e-005 -4.999 -4.999 0.000

CaOH+ 1.638e-007 1.526e-007 -6.786 -6.816 -0.031

CaHSO4+ 4.758e-014 4.433e-014 -13.323 -13.353 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.333e-005 -4.242 -4.273 -0.031

H(0) 6.354e-030

H2 3.177e-030 3.180e-030 -29.498 -29.498 0.000

K 3.326e-006

K+ 3.324e-006 3.095e-006 -5.478 -5.509 -0.031

KSO4- 1.942e-009 1.810e-009 -8.712 -8.742 -0.031

KOH 1.549e-011 1.551e-011 -10.810 -10.809 0.000

Mg 5.184e-004

Mg+2 4.491e-004 3.418e-004 -3.348 -3.466 -0.119

MgCO3 5.069e-005 5.074e-005 -4.295 -4.295 0.000

MgHCO3+ 8.166e-006 7.609e-006 -5.088 -5.119 -0.031

MgSO4 7.025e-006 7.031e-006 -5.153 -5.153 0.000

MgOH+ 3.425e-006 3.191e-006 -5.465 -5.496 -0.031

Na 1.001e-005

Na+ 9.957e-006 9.284e-006 -5.002 -5.032 -0.030

NaCO3- 3.602e-008 3.357e-008 -7.443 -7.474 -0.031

NaHCO3 9.599e-009 9.608e-009 -8.018 -8.017 0.000

NaSO4- 3.871e-009 3.607e-009 -8.412 -8.443 -0.031

NaOH 8.857e-011 8.865e-011 -10.053 -10.052 0.000

O(0) 1.353e-003

O2 6.767e-004 6.774e-004 -3.170 -3.169 0.000

S(6) 1.154e-004

SO4-2 9.832e-005 7.446e-005 -4.007 -4.128 -0.121

CaSO4 1.002e-005 1.003e-005 -4.999 -4.999 0.000

MgSO4 7.025e-006 7.031e-006 -5.153 -5.153 0.000

NaSO4- 3.871e-009 3.607e-009 -8.412 -8.443 -0.031

KSO4- 1.942e-009 1.810e-009 -8.712 -8.742 -0.031

HSO4- 6.219e-012 5.795e-012 -11.206 -11.237 -0.031

CaHSO4+ 4.758e-014 4.433e-014 -13.323 -13.353 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.93 -7.32 -4.39 CaSO4

Aragonite 1.33 -7.05 -8.38 CaCO3

Calcite 1.47 -7.05 -8.52 CaCO3

CO2(g) -4.03 -5.57 -1.54 CO2

Dolomite 2.87 -14.37 -17.24 CaMg(CO3)2

Gypsum -2.74 -7.32 -4.59 CaSO4:2H2O

H2(g) -26.32 -29.50 -3.18 H2

H2O(g) -1.34 -0.00 1.34 H2O

Halite -10.90 -9.31 1.60 NaCl

O2(g) -0.23 -3.17 -2.94 O2

Initial solution 110. 30/8/2012 15:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.866e-003 2.866e-003

Ca 1.047e-003 1.047e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.335e-003 1.335e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.150

pe = 4.000

Specific Conductance (uS/cm, 31 oC) = 306

Density (g/cm3) = 0.99534

Activity of water = 1.000

Ionic strength = 4.214e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.433e-003

Total CO2 (mol/kg) = 2.433e-003

Temperature (deg C) = 31.650

Electrical balance (eq) = -9.272e-006

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.18

Iterations = 7

Total H = 1.110145e+002

Total O = 5.551534e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.0373 0.6675

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.470e-005 2.299e-005 -4.607 -4.639 -0.031

H+ 7.552e-010 7.079e-010 -9.122 -9.150 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.433e-003

HCO3- 1.996e-003 1.862e-003 -2.700 -2.730 -0.030

CO3-2 1.839e-004 1.395e-004 -3.736 -3.855 -0.120

CaCO3 1.740e-004 1.741e-004 -3.760 -3.759 0.000

MgCO3 5.033e-005 5.038e-005 -4.298 -4.298 0.000

CaHCO3+ 1.782e-005 1.663e-005 -4.749 -4.779 -0.030

MgHCO3+ 8.271e-006 7.705e-006 -5.082 -5.113 -0.031

CO2 2.762e-006 2.765e-006 -5.559 -5.558 0.000

NaCO3- 3.593e-008 3.347e-008 -7.445 -7.475 -0.031

NaHCO3 9.712e-009 9.721e-009 -8.013 -8.012 0.000

Ca 1.047e-003

Ca+2 8.454e-004 6.410e-004 -3.073 -3.193 -0.120

CaCO3 1.740e-004 1.741e-004 -3.760 -3.759 0.000

CaHCO3+ 1.782e-005 1.663e-005 -4.749 -4.779 -0.030

CaSO4 1.009e-005 1.010e-005 -4.996 -4.996 0.000

CaOH+ 1.613e-007 1.503e-007 -6.792 -6.823 -0.031

CaHSO4+ 4.912e-014 4.577e-014 -13.309 -13.339 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.332e-005 -4.242 -4.273 -0.031

H(0) 6.645e-030

H2 3.322e-030 3.326e-030 -29.479 -29.478 0.000

K 3.326e-006

K+ 3.324e-006 3.094e-006 -5.478 -5.509 -0.031

KSO4- 1.943e-009 1.810e-009 -8.711 -8.742 -0.031

KOH 1.514e-011 1.515e-011 -10.820 -10.819 0.000

Mg 5.184e-004

Mg+2 4.494e-004 3.418e-004 -3.347 -3.466 -0.119

MgCO3 5.033e-005 5.038e-005 -4.298 -4.298 0.000

MgHCO3+ 8.271e-006 7.705e-006 -5.082 -5.113 -0.031

MgSO4 7.035e-006 7.042e-006 -5.153 -5.152 0.000

MgOH+ 3.385e-006 3.154e-006 -5.470 -5.501 -0.031

Na 1.001e-005

Na+ 9.957e-006 9.282e-006 -5.002 -5.032 -0.030

NaCO3- 3.593e-008 3.347e-008 -7.445 -7.475 -0.031

NaHCO3 9.712e-009 9.721e-009 -8.013 -8.012 0.000

NaSO4- 3.868e-009 3.604e-009 -8.412 -8.443 -0.031

NaOH 8.654e-011 8.662e-011 -10.063 -10.062 0.000

O(0) 1.335e-003

O2 6.674e-004 6.680e-004 -3.176 -3.175 0.000

S(6) 1.154e-004

SO4-2 9.824e-005 7.434e-005 -4.008 -4.129 -0.121

CaSO4 1.009e-005 1.010e-005 -4.996 -4.996 0.000

MgSO4 7.035e-006 7.042e-006 -5.153 -5.152 0.000

NaSO4- 3.868e-009 3.604e-009 -8.412 -8.443 -0.031

KSO4- 1.943e-009 1.810e-009 -8.711 -8.742 -0.031

HSO4- 6.374e-012 5.938e-012 -11.196 -11.226 -0.031

CaHSO4+ 4.912e-014 4.577e-014 -13.309 -13.339 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.93 -7.32 -4.40 CaSO4

Aragonite 1.33 -7.05 -8.38 CaCO3

Calcite 1.47 -7.05 -8.52 CaCO3

CO2(g) -4.02 -5.56 -1.54 CO2

Dolomite 2.87 -14.37 -17.24 CaMg(CO3)2

Gypsum -2.74 -7.32 -4.59 CaSO4:2H2O

H2(g) -26.30 -29.48 -3.18 H2

H2O(g) -1.34 -0.00 1.34 H2O

Halite -10.90 -9.31 1.60 NaCl

O2(g) -0.24 -3.18 -2.94 O2

Initial solution 111. 30/8/2012 15:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.835e-003 2.835e-003

Ca 1.036e-003 1.036e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.375e-003 1.375e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.170

pe = 4.000

Specific Conductance (uS/cm, 31 oC) = 303

Density (g/cm3) = 0.99531

Activity of water = 1.000

Ionic strength = 4.172e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.392e-003

Total CO2 (mol/kg) = 2.392e-003

Temperature (deg C) = 31.740

Electrical balance (eq) = -7.505e-007

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.01

Iterations = 7

Total H = 1.110144e+002

Total O = 5.551526e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.0134 0.6662

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.602e-005 2.422e-005 -4.585 -4.616 -0.031

H+ 7.210e-010 6.761e-010 -9.142 -9.170 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.392e-003

HCO3- 1.949e-003 1.819e-003 -2.710 -2.740 -0.030

CO3-2 1.881e-004 1.429e-004 -3.726 -3.845 -0.119

CaCO3 1.761e-004 1.763e-004 -3.754 -3.754 0.000

MgCO3 5.155e-005 5.160e-005 -4.288 -4.287 0.000

CaHCO3+ 1.718e-005 1.604e-005 -4.765 -4.795 -0.030

MgHCO3+ 8.068e-006 7.519e-006 -5.093 -5.124 -0.031

CO2 2.575e-006 2.577e-006 -5.589 -5.589 0.000

NaCO3- 3.696e-008 3.444e-008 -7.432 -7.463 -0.031

NaHCO3 9.488e-009 9.498e-009 -8.023 -8.022 0.000

Ca 1.036e-003

Ca+2 8.327e-004 6.322e-004 -3.079 -3.199 -0.120

CaCO3 1.761e-004 1.763e-004 -3.754 -3.754 0.000

CaHCO3+ 1.718e-005 1.604e-005 -4.765 -4.795 -0.030

CaSO4 9.984e-006 9.994e-006 -5.001 -5.000 0.000

CaOH+ 1.665e-007 1.552e-007 -6.779 -6.809 -0.031

CaHSO4+ 4.645e-014 4.328e-014 -13.333 -13.364 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.334e-005 -4.242 -4.273 -0.031

H(0) 6.055e-030

H2 3.027e-030 3.030e-030 -29.519 -29.519 0.000

K 3.326e-006

K+ 3.324e-006 3.095e-006 -5.478 -5.509 -0.031

KSO4- 1.950e-009 1.818e-009 -8.710 -8.740 -0.031

KOH 1.586e-011 1.587e-011 -10.800 -10.799 0.000

Mg 5.184e-004

Mg+2 4.482e-004 3.412e-004 -3.349 -3.467 -0.118

MgCO3 5.155e-005 5.160e-005 -4.288 -4.287 0.000

MgHCO3+ 8.068e-006 7.519e-006 -5.093 -5.124 -0.031

MgSO4 7.055e-006 7.062e-006 -5.151 -5.151 0.000

MgOH+ 3.566e-006 3.323e-006 -5.448 -5.478 -0.031

Na 1.001e-005

Na+ 9.957e-006 9.284e-006 -5.002 -5.032 -0.030

NaCO3- 3.696e-008 3.444e-008 -7.432 -7.463 -0.031

NaHCO3 9.488e-009 9.498e-009 -8.023 -8.022 0.000

NaSO4- 3.879e-009 3.614e-009 -8.411 -8.442 -0.031

NaOH 9.064e-011 9.072e-011 -10.043 -10.042 0.000

O(0) 1.375e-003

O2 6.874e-004 6.880e-004 -3.163 -3.162 0.000

S(6) 1.154e-004

SO4-2 9.832e-005 7.450e-005 -4.007 -4.128 -0.121

CaSO4 9.984e-006 9.994e-006 -5.001 -5.000 0.000

MgSO4 7.055e-006 7.062e-006 -5.151 -5.151 0.000

NaSO4- 3.879e-009 3.614e-009 -8.411 -8.442 -0.031

KSO4- 1.950e-009 1.818e-009 -8.710 -8.740 -0.031

HSO4- 6.111e-012 5.695e-012 -11.214 -11.245 -0.031

CaHSO4+ 4.645e-014 4.328e-014 -13.333 -13.364 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.93 -7.33 -4.40 CaSO4

Aragonite 1.34 -7.04 -8.38 CaCO3

Calcite 1.48 -7.04 -8.52 CaCO3

CO2(g) -4.05 -5.59 -1.54 CO2

Dolomite 2.89 -14.36 -17.24 CaMg(CO3)2

Gypsum -2.74 -7.33 -4.59 CaSO4:2H2O

H2(g) -26.34 -29.52 -3.18 H2

H2O(g) -1.34 -0.00 1.34 H2O

Halite -10.90 -9.31 1.60 NaCl

O2(g) -0.22 -3.16 -2.94 O2

Initial solution 112. 30/8/2012 15:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.835e-003 2.835e-003

Ca 1.036e-003 1.036e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.363e-003 1.363e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.140

pe = 4.000

Specific Conductance (uS/cm, 31 oC) = 305

Density (g/cm3) = 0.99530

Activity of water = 1.000

Ionic strength = 4.189e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.413e-003

Total CO2 (mol/kg) = 2.413e-003

Temperature (deg C) = 31.780

Electrical balance (eq) = -7.505e-007

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.01

Iterations = 7

Total H = 1.110145e+002

Total O = 5.551530e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.0393 0.6679

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.435e-005 2.267e-005 -4.613 -4.645 -0.031

H+ 7.727e-010 7.244e-010 -9.112 -9.140 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.413e-003

HCO3- 1.986e-003 1.854e-003 -2.702 -2.732 -0.030

CO3-2 1.791e-004 1.360e-004 -3.747 -3.866 -0.120

CaCO3 1.691e-004 1.692e-004 -3.772 -3.772 0.000

MgCO3 4.932e-005 4.936e-005 -4.307 -4.307 0.000

CaHCO3+ 1.765e-005 1.648e-005 -4.753 -4.783 -0.030

MgHCO3+ 8.263e-006 7.699e-006 -5.083 -5.114 -0.031

CO2 2.811e-006 2.814e-006 -5.551 -5.551 0.000

NaCO3- 3.525e-008 3.285e-008 -7.453 -7.483 -0.031

NaHCO3 9.671e-009 9.681e-009 -8.015 -8.014 0.000

Ca 1.036e-003

Ca+2 8.393e-004 6.368e-004 -3.076 -3.196 -0.120

CaCO3 1.691e-004 1.692e-004 -3.772 -3.772 0.000

CaHCO3+ 1.765e-005 1.648e-005 -4.753 -4.783 -0.030

CaSO4 1.005e-005 1.006e-005 -4.998 -4.998 0.000

CaOH+ 1.566e-007 1.459e-007 -6.805 -6.836 -0.031

CaHSO4+ 5.011e-014 4.669e-014 -13.300 -13.331 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.333e-005 -4.242 -4.273 -0.031

H(0) 6.949e-030

H2 3.475e-030 3.478e-030 -29.459 -29.459 0.000

K 3.326e-006

K+ 3.324e-006 3.095e-006 -5.478 -5.509 -0.031

KSO4- 1.949e-009 1.816e-009 -8.710 -8.741 -0.031

KOH 1.480e-011 1.481e-011 -10.830 -10.829 0.000

Mg 5.184e-004

Mg+2 4.504e-004 3.428e-004 -3.346 -3.465 -0.119

MgCO3 4.932e-005 4.936e-005 -4.307 -4.307 0.000

MgHCO3+ 8.263e-006 7.699e-006 -5.083 -5.114 -0.031

MgSO4 7.083e-006 7.090e-006 -5.150 -5.149 0.000

MgOH+ 3.354e-006 3.126e-006 -5.474 -5.505 -0.031

Na 1.001e-005

Na+ 9.958e-006 9.284e-006 -5.002 -5.032 -0.030

NaCO3- 3.525e-008 3.285e-008 -7.453 -7.483 -0.031

NaHCO3 9.671e-009 9.681e-009 -8.015 -8.014 0.000

NaSO4- 3.874e-009 3.610e-009 -8.412 -8.442 -0.031

NaOH 8.459e-011 8.467e-011 -10.073 -10.072 0.000

O(0) 1.363e-003

O2 6.814e-004 6.821e-004 -3.167 -3.166 0.000

S(6) 1.154e-004

SO4-2 9.824e-005 7.439e-005 -4.008 -4.128 -0.121

CaSO4 1.005e-005 1.006e-005 -4.998 -4.998 0.000

MgSO4 7.083e-006 7.090e-006 -5.150 -5.149 0.000

NaSO4- 3.874e-009 3.610e-009 -8.412 -8.442 -0.031

KSO4- 1.949e-009 1.816e-009 -8.710 -8.741 -0.031

HSO4- 6.545e-012 6.099e-012 -11.184 -11.215 -0.031

CaHSO4+ 5.011e-014 4.669e-014 -13.300 -13.331 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.93 -7.32 -4.40 CaSO4

Aragonite 1.32 -7.06 -8.38 CaCO3

Calcite 1.46 -7.06 -8.52 CaCO3

CO2(g) -4.01 -5.55 -1.54 CO2

Dolomite 2.85 -14.39 -17.24 CaMg(CO3)2

Gypsum -2.74 -7.32 -4.59 CaSO4:2H2O

H2(g) -26.28 -29.46 -3.18 H2

H2O(g) -1.34 -0.00 1.34 H2O

Halite -10.90 -9.31 1.60 NaCl

O2(g) -0.23 -3.17 -2.94 O2

Initial solution 113. 30/8/2012 16:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.814e-003 2.814e-003

Ca 1.029e-003 1.029e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.332e-003 1.332e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.150

pe = 4.000

Specific Conductance (uS/cm, 31 oC) = 303

Density (g/cm3) = 0.99530

Activity of water = 1.000

Ionic strength = 4.164e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.389e-003

Total CO2 (mol/kg) = 2.389e-003

Temperature (deg C) = 31.790

Electrical balance (eq) = 5.094e-006

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.10

Iterations = 7

Total H = 1.110144e+002

Total O = 5.551520e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.0260 0.6671

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.493e-005 2.322e-005 -4.603 -4.634 -0.031

H+ 7.550e-010 7.079e-010 -9.122 -9.150 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.389e-003

HCO3- 1.960e-003 1.830e-003 -2.708 -2.738 -0.030

CO3-2 1.808e-004 1.374e-004 -3.743 -3.862 -0.119

CaCO3 1.694e-004 1.696e-004 -3.771 -3.771 0.000

MgCO3 4.981e-005 4.986e-005 -4.303 -4.302 0.000

CaHCO3+ 1.728e-005 1.613e-005 -4.762 -4.792 -0.030

MgHCO3+ 8.152e-006 7.597e-006 -5.089 -5.119 -0.031

CO2 2.711e-006 2.714e-006 -5.567 -5.566 0.000

NaCO3- 3.563e-008 3.320e-008 -7.448 -7.479 -0.031

NaHCO3 9.547e-009 9.557e-009 -8.020 -8.020 0.000

Ca 1.029e-003

Ca+2 8.319e-004 6.316e-004 -3.080 -3.200 -0.120

CaCO3 1.694e-004 1.696e-004 -3.771 -3.771 0.000

CaHCO3+ 1.728e-005 1.613e-005 -4.762 -4.792 -0.030

CaSO4 9.979e-006 9.988e-006 -5.001 -5.001 0.000

CaOH+ 1.589e-007 1.481e-007 -6.799 -6.830 -0.031

CaHSO4+ 4.864e-014 4.533e-014 -13.313 -13.344 -0.031

Cl 5.727e-005

Cl- 5.727e-005 5.334e-005 -4.242 -4.273 -0.031

H(0) 6.636e-030

H2 3.318e-030 3.321e-030 -29.479 -29.479 0.000

K 3.326e-006

K+ 3.324e-006 3.095e-006 -5.478 -5.509 -0.031

KSO4- 1.952e-009 1.819e-009 -8.710 -8.740 -0.031

KOH 1.514e-011 1.516e-011 -10.820 -10.819 0.000

Mg 5.184e-004

Mg+2 4.499e-004 3.426e-004 -3.347 -3.465 -0.118

MgCO3 4.981e-005 4.986e-005 -4.303 -4.302 0.000

MgHCO3+ 8.152e-006 7.597e-006 -5.089 -5.119 -0.031

MgSO4 7.092e-006 7.099e-006 -5.149 -5.149 0.000

MgOH+ 3.434e-006 3.200e-006 -5.464 -5.495 -0.031

Na 1.001e-005

Na+ 9.958e-006 9.286e-006 -5.002 -5.032 -0.030

NaCO3- 3.563e-008 3.320e-008 -7.448 -7.479 -0.031

NaHCO3 9.547e-009 9.557e-009 -8.020 -8.020 0.000

NaSO4- 3.880e-009 3.616e-009 -8.411 -8.442 -0.031

NaOH 8.657e-011 8.665e-011 -10.063 -10.062 0.000

O(0) 1.332e-003

O2 6.661e-004 6.667e-004 -3.176 -3.176 0.000

S(6) 1.154e-004

SO4-2 9.829e-005 7.449e-005 -4.007 -4.128 -0.120

CaSO4 9.979e-006 9.988e-006 -5.001 -5.001 0.000

MgSO4 7.092e-006 7.099e-006 -5.149 -5.149 0.000

NaSO4- 3.880e-009 3.616e-009 -8.411 -8.442 -0.031

KSO4- 1.952e-009 1.819e-009 -8.710 -8.740 -0.031

HSO4- 6.405e-012 5.969e-012 -11.193 -11.224 -0.031

CaHSO4+ 4.864e-014 4.533e-014 -13.313 -13.344 -0.031

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.93 -7.33 -4.40 CaSO4

Aragonite 1.32 -7.06 -8.38 CaCO3

Calcite 1.46 -7.06 -8.52 CaCO3

CO2(g) -4.02 -5.57 -1.54 CO2

Dolomite 2.86 -14.39 -17.24 CaMg(CO3)2

Gypsum -2.74 -7.33 -4.59 CaSO4:2H2O

H2(g) -26.30 -29.48 -3.18 H2

H2O(g) -1.34 -0.00 1.34 H2O

Halite -10.90 -9.31 1.60 NaCl

O2(g) -0.24 -3.18 -2.94 O2

Initial solution 114. 30/8/2012 16:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.773e-003 2.773e-003

Ca 1.014e-003 1.014e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.353e-003 1.353e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.150

pe = 4.000

Specific Conductance (uS/cm, 31 oC) = 300

Density (g/cm3) = 0.99531

Activity of water = 1.000

Ionic strength = 4.127e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.355e-003

Total CO2 (mol/kg) = 2.355e-003

Temperature (deg C) = 31.740

Electrical balance (eq) = 1.646e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.32

Iterations = 7

Total H = 1.110144e+002

Total O = 5.551512e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.0317 0.6673

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.484e-005 2.313e-005 -4.605 -4.636 -0.031

H+ 7.548e-010 7.079e-010 -9.122 -9.150 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.355e-003

HCO3- 1.935e-003 1.807e-003 -2.713 -2.743 -0.030

CO3-2 1.782e-004 1.355e-004 -3.749 -3.868 -0.119

CaCO3 1.651e-004 1.652e-004 -3.782 -3.782 0.000

MgCO3 4.922e-005 4.927e-005 -4.308 -4.307 0.000

CaHCO3+ 1.686e-005 1.574e-005 -4.773 -4.803 -0.030

MgHCO3+ 8.064e-006 7.517e-006 -5.093 -5.124 -0.030

CO2 2.678e-006 2.680e-006 -5.572 -5.572 0.000

NaCO3- 3.506e-008 3.269e-008 -7.455 -7.486 -0.030

NaHCO3 9.429e-009 9.438e-009 -8.026 -8.025 0.000

Ca 1.014e-003

Ca+2 8.218e-004 6.247e-004 -3.085 -3.204 -0.119

CaCO3 1.651e-004 1.652e-004 -3.782 -3.782 0.000

CaHCO3+ 1.686e-005 1.574e-005 -4.773 -4.803 -0.030

CaSO4 9.883e-006 9.892e-006 -5.005 -5.005 0.000

CaOH+ 1.571e-007 1.464e-007 -6.804 -6.834 -0.030

CaHSO4+ 4.813e-014 4.487e-014 -13.318 -13.348 -0.030

Cl 5.727e-005

Cl- 5.727e-005 5.336e-005 -4.242 -4.273 -0.031

H(0) 6.639e-030

H2 3.320e-030 3.323e-030 -29.479 -29.479 0.000

K 3.325e-006

K+ 3.324e-006 3.096e-006 -5.478 -5.509 -0.031

KSO4- 1.954e-009 1.821e-009 -8.709 -8.740 -0.030

KOH 1.515e-011 1.516e-011 -10.820 -10.819 0.000

Mg 5.184e-004

Mg+2 4.506e-004 3.435e-004 -3.346 -3.464 -0.118

MgCO3 4.922e-005 4.927e-005 -4.308 -4.307 0.000

MgHCO3+ 8.064e-006 7.517e-006 -5.093 -5.124 -0.030

MgSO4 7.115e-006 7.122e-006 -5.148 -5.147 0.000

MgOH+ 3.427e-006 3.194e-006 -5.465 -5.496 -0.030

Na 1.001e-005

Na+ 9.959e-006 9.289e-006 -5.002 -5.032 -0.030

NaCO3- 3.506e-008 3.269e-008 -7.455 -7.486 -0.030

NaHCO3 9.429e-009 9.438e-009 -8.026 -8.025 0.000

NaSO4- 3.886e-009 3.623e-009 -8.410 -8.441 -0.030

NaOH 8.660e-011 8.669e-011 -10.062 -10.062 0.000

O(0) 1.353e-003

O2 6.767e-004 6.774e-004 -3.170 -3.169 0.000

S(6) 1.154e-004

SO4-2 9.837e-005 7.463e-005 -4.007 -4.127 -0.120

CaSO4 9.883e-006 9.892e-006 -5.005 -5.005 0.000

MgSO4 7.115e-006 7.122e-006 -5.148 -5.147 0.000

NaSO4- 3.886e-009 3.623e-009 -8.410 -8.441 -0.030

KSO4- 1.954e-009 1.821e-009 -8.709 -8.740 -0.030

HSO4- 6.408e-012 5.974e-012 -11.193 -11.224 -0.030

CaHSO4+ 4.813e-014 4.487e-014 -13.318 -13.348 -0.030

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.94 -7.33 -4.40 CaSO4

Aragonite 1.31 -7.07 -8.38 CaCO3

Calcite 1.45 -7.07 -8.52 CaCO3

CO2(g) -4.03 -5.57 -1.54 CO2

Dolomite 2.84 -14.40 -17.24 CaMg(CO3)2

Gypsum -2.75 -7.33 -4.59 CaSO4:2H2O

H2(g) -26.30 -29.48 -3.18 H2

H2O(g) -1.34 -0.00 1.34 H2O

Halite -10.90 -9.30 1.60 NaCl

O2(g) -0.23 -3.17 -2.94 O2

Initial solution 115. 30/8/2012 16:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.732e-003 2.732e-003

Ca 9.988e-004 9.988e-004

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.356e-003 1.356e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.200

pe = 4.000

Specific Conductance (uS/cm, 31 oC) = 294

Density (g/cm3) = 0.99537

Activity of water = 1.000

Ionic strength = 4.063e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.289e-003

Total CO2 (mol/kg) = 2.289e-003

Temperature (deg C) = 31.530

Electrical balance (eq) = 2.765e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.55

Iterations = 7

Total H = 1.110143e+002

Total O = 5.551493e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 10.9986 0.6649

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.744e-005 2.557e-005 -4.562 -4.592 -0.031

H+ 6.724e-010 6.310e-010 -9.172 -9.200 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.289e-003

HCO3- 1.849e-003 1.728e-003 -2.733 -2.763 -0.029

CO3-2 1.901e-004 1.449e-004 -3.721 -3.839 -0.118

CaCO3 1.716e-004 1.718e-004 -3.765 -3.765 0.000

MgCO3 5.222e-005 5.227e-005 -4.282 -4.282 0.000

CaHCO3+ 1.571e-005 1.468e-005 -4.804 -4.833 -0.029

MgHCO3+ 7.663e-006 7.148e-006 -5.116 -5.146 -0.030

CO2 2.286e-006 2.289e-006 -5.641 -5.640 0.000

NaCO3- 3.710e-008 3.461e-008 -7.431 -7.461 -0.030

NaHCO3 9.020e-009 9.028e-009 -8.045 -8.044 0.000

Ca 9.988e-004

Ca+2 8.016e-004 6.106e-004 -3.096 -3.214 -0.118

CaCO3 1.716e-004 1.718e-004 -3.765 -3.765 0.000

CaHCO3+ 1.571e-005 1.468e-005 -4.804 -4.833 -0.029

CaSO4 9.684e-006 9.693e-006 -5.014 -5.014 0.000

CaOH+ 1.722e-007 1.606e-007 -6.764 -6.794 -0.030

CaHSO4+ 4.188e-014 3.907e-014 -13.378 -13.408 -0.030

Cl 5.727e-005

Cl- 5.727e-005 5.339e-005 -4.242 -4.273 -0.031

H(0) 5.284e-030

H2 2.642e-030 2.645e-030 -29.578 -29.578 0.000

K 3.325e-006

K+ 3.324e-006 3.098e-006 -5.478 -5.509 -0.031

KSO4- 1.956e-009 1.824e-009 -8.709 -8.739 -0.030

KOH 1.701e-011 1.702e-011 -10.769 -10.769 0.000

Mg 5.184e-004

Mg+2 4.477e-004 3.420e-004 -3.349 -3.466 -0.117

MgCO3 5.222e-005 5.227e-005 -4.282 -4.282 0.000

MgHCO3+ 7.663e-006 7.148e-006 -5.116 -5.146 -0.030

MgSO4 7.078e-006 7.085e-006 -5.150 -5.150 0.000

MgOH+ 3.757e-006 3.504e-006 -5.425 -5.455 -0.030

Na 1.001e-005

Na+ 9.957e-006 9.292e-006 -5.002 -5.032 -0.030

NaCO3- 3.710e-008 3.461e-008 -7.431 -7.461 -0.030

NaHCO3 9.020e-009 9.028e-009 -8.045 -8.044 0.000

NaSO4- 3.898e-009 3.636e-009 -8.409 -8.439 -0.030

NaOH 9.721e-011 9.730e-011 -10.012 -10.012 0.000

O(0) 1.356e-003

O2 6.780e-004 6.786e-004 -3.169 -3.168 0.000

S(6) 1.154e-004

SO4-2 9.860e-005 7.496e-005 -4.006 -4.125 -0.119

CaSO4 9.684e-006 9.693e-006 -5.014 -5.014 0.000

MgSO4 7.078e-006 7.085e-006 -5.150 -5.150 0.000

NaSO4- 3.898e-009 3.636e-009 -8.409 -8.439 -0.030

KSO4- 1.956e-009 1.824e-009 -8.709 -8.739 -0.030

HSO4- 5.706e-012 5.322e-012 -11.244 -11.274 -0.030

CaHSO4+ 4.188e-014 3.907e-014 -13.378 -13.408 -0.030

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.94 -7.34 -4.39 CaSO4

Aragonite 1.33 -7.05 -8.38 CaCO3

Calcite 1.47 -7.05 -8.52 CaCO3

CO2(g) -4.10 -5.64 -1.54 CO2

Dolomite 2.88 -14.36 -17.24 CaMg(CO3)2

Gypsum -2.75 -7.34 -4.59 CaSO4:2H2O

H2(g) -26.40 -29.58 -3.18 H2

H2O(g) -1.34 -0.00 1.34 H2O

Halite -10.90 -9.30 1.60 NaCl

O2(g) -0.23 -3.17 -2.94 O2

Initial solution 116. 30/8/2012 16:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.701e-003 2.701e-003

Ca 9.875e-004 9.875e-004

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.330e-003 1.330e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.180

pe = 4.000

Specific Conductance (uS/cm, 31 oC) = 291

Density (g/cm3) = 0.99547

Activity of water = 1.000

Ionic strength = 4.052e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.280e-003

Total CO2 (mol/kg) = 2.280e-003

Temperature (deg C) = 31.210

Electrical balance (eq) = 3.617e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.72

Iterations = 7

Total H = 1.110143e+002

Total O = 5.551488e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.0418 0.6668

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.562e-005 2.388e-005 -4.591 -4.622 -0.031

H+ 7.040e-010 6.607e-010 -9.152 -9.180 -0.028

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.280e-003

HCO3- 1.860e-003 1.738e-003 -2.730 -2.760 -0.029

CO3-2 1.816e-004 1.385e-004 -3.741 -3.859 -0.118

CaCO3 1.624e-004 1.626e-004 -3.789 -3.789 0.000

MgCO3 4.996e-005 5.000e-005 -4.301 -4.301 0.000

CaHCO3+ 1.571e-005 1.468e-005 -4.804 -4.833 -0.029

MgHCO3+ 7.741e-006 7.221e-006 -5.111 -5.141 -0.030

CO2 2.416e-006 2.418e-006 -5.617 -5.617 0.000

NaCO3- 3.492e-008 3.257e-008 -7.457 -7.487 -0.030

NaHCO3 9.078e-009 9.086e-009 -8.042 -8.042 0.000

Ca 9.875e-004

Ca+2 7.996e-004 6.093e-004 -3.097 -3.215 -0.118

CaCO3 1.624e-004 1.626e-004 -3.789 -3.789 0.000

CaHCO3+ 1.571e-005 1.468e-005 -4.804 -4.833 -0.029

CaSO4 9.647e-006 9.656e-006 -5.016 -5.015 0.000

CaOH+ 1.641e-007 1.530e-007 -6.785 -6.815 -0.030

CaHSO4+ 4.349e-014 4.057e-014 -13.362 -13.392 -0.030

Cl 5.727e-005

Cl- 5.727e-005 5.339e-005 -4.242 -4.273 -0.030

H(0) 5.812e-030

H2 2.906e-030 2.909e-030 -29.537 -29.536 0.000

K 3.325e-006

K+ 3.324e-006 3.098e-006 -5.478 -5.509 -0.030

KSO4- 1.947e-009 1.816e-009 -8.711 -8.741 -0.030

KOH 1.624e-011 1.626e-011 -10.789 -10.789 0.000

Mg 5.184e-004

Mg+2 4.501e-004 3.440e-004 -3.347 -3.463 -0.117

MgCO3 4.996e-005 5.000e-005 -4.301 -4.301 0.000

MgHCO3+ 7.741e-006 7.221e-006 -5.111 -5.141 -0.030

MgSO4 7.071e-006 7.078e-006 -5.151 -5.150 0.000

MgOH+ 3.510e-006 3.274e-006 -5.455 -5.485 -0.030

Na 1.001e-005

Na+ 9.959e-006 9.296e-006 -5.002 -5.032 -0.030

NaCO3- 3.492e-008 3.257e-008 -7.457 -7.487 -0.030

NaHCO3 9.078e-009 9.086e-009 -8.042 -8.042 0.000

NaSO4- 3.895e-009 3.633e-009 -8.410 -8.440 -0.030

NaOH 9.286e-011 9.295e-011 -10.032 -10.032 0.000

O(0) 1.330e-003

O2 6.649e-004 6.655e-004 -3.177 -3.177 0.000

S(6) 1.154e-004

SO4-2 9.865e-005 7.503e-005 -4.006 -4.125 -0.119

CaSO4 9.647e-006 9.656e-006 -5.016 -5.015 0.000

MgSO4 7.071e-006 7.078e-006 -5.151 -5.150 0.000

NaSO4- 3.895e-009 3.633e-009 -8.410 -8.440 -0.030

KSO4- 1.947e-009 1.816e-009 -8.711 -8.741 -0.030

HSO4- 5.936e-012 5.538e-012 -11.226 -11.257 -0.030

CaHSO4+ 4.349e-014 4.057e-014 -13.362 -13.392 -0.030

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.95 -7.34 -4.39 CaSO4

Aragonite 1.30 -7.07 -8.38 CaCO3

Calcite 1.44 -7.07 -8.52 CaCO3

CO2(g) -4.08 -5.62 -1.54 CO2

Dolomite 2.84 -14.40 -17.23 CaMg(CO3)2

Gypsum -2.76 -7.34 -4.58 CaSO4:2H2O

H2(g) -26.36 -29.54 -3.18 H2

H2O(g) -1.35 -0.00 1.35 H2O

Halite -10.90 -9.30 1.60 NaCl

O2(g) -0.24 -3.18 -2.93 O2

Initial solution 117. 30/8/2012 17:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.556e-003 2.556e-003

Ca 9.351e-004 9.351e-004

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.336e-003 1.336e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.240

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 278

Density (g/cm3) = 0.99557

Activity of water = 1.000

Ionic strength = 3.891e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.125e-003

Total CO2 (mol/kg) = 2.125e-003

Temperature (deg C) = 30.860

Electrical balance (eq) = 7.610e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 1.58

Iterations = 6

Total H = 1.110142e+002

Total O = 5.551442e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.0102 0.6641

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.865e-005 2.674e-005 -4.543 -4.573 -0.030

H+ 6.125e-010 5.754e-010 -9.213 -9.240 -0.027

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.125e-003

HCO3- 1.702e-003 1.593e-003 -2.769 -2.798 -0.029

CO3-2 1.889e-004 1.448e-004 -3.724 -3.839 -0.116

CaCO3 1.594e-004 1.595e-004 -3.798 -3.797 0.000

MgCO3 5.201e-005 5.205e-005 -4.284 -4.284 0.000

CaHCO3+ 1.355e-005 1.268e-005 -4.868 -4.897 -0.029

MgHCO3+ 7.075e-006 6.609e-006 -5.150 -5.180 -0.030

CO2 1.934e-006 1.935e-006 -5.714 -5.713 0.000

NaCO3- 3.590e-008 3.353e-008 -7.445 -7.475 -0.030

NaHCO3 8.328e-009 8.335e-009 -8.079 -8.079 0.000

Ca 9.351e-004

Ca+2 7.528e-004 5.766e-004 -3.123 -3.239 -0.116

CaCO3 1.594e-004 1.595e-004 -3.798 -3.797 0.000

CaHCO3+ 1.355e-005 1.268e-005 -4.868 -4.897 -0.029

CaSO4 9.188e-006 9.197e-006 -5.037 -5.036 0.000

CaOH+ 1.780e-007 1.663e-007 -6.750 -6.779 -0.030

CaHSO4+ 3.585e-014 3.349e-014 -13.445 -13.475 -0.030

Cl 5.727e-005

Cl- 5.727e-005 5.346e-005 -4.242 -4.272 -0.030

H(0) 4.424e-030

H2 2.212e-030 2.214e-030 -29.655 -29.655 0.000

K 3.325e-006

K+ 3.323e-006 3.102e-006 -5.478 -5.508 -0.030

KSO4- 1.954e-009 1.826e-009 -8.709 -8.739 -0.030

KOH 1.868e-011 1.869e-011 -10.729 -10.728 0.000

Mg 5.184e-004

Mg+2 4.483e-004 3.443e-004 -3.348 -3.463 -0.115

MgCO3 5.201e-005 5.205e-005 -4.284 -4.284 0.000

MgSO4 7.085e-006 7.091e-006 -5.150 -5.149 0.000

MgHCO3+ 7.075e-006 6.609e-006 -5.150 -5.180 -0.030

MgOH+ 3.908e-006 3.650e-006 -5.408 -5.438 -0.030

Na 1.001e-005

Na+ 9.959e-006 9.307e-006 -5.002 -5.031 -0.029

NaCO3- 3.590e-008 3.353e-008 -7.445 -7.475 -0.030

NaHCO3 8.328e-009 8.335e-009 -8.079 -8.079 0.000

NaSO4- 3.924e-009 3.665e-009 -8.406 -8.436 -0.030

NaOH 1.068e-010 1.069e-010 -9.972 -9.971 0.000

O(0) 1.336e-003

O2 6.680e-004 6.686e-004 -3.175 -3.175 0.000

S(6) 1.154e-004

SO4-2 9.909e-005 7.576e-005 -4.004 -4.121 -0.117

CaSO4 9.188e-006 9.197e-006 -5.037 -5.036 0.000

MgSO4 7.085e-006 7.091e-006 -5.150 -5.149 0.000

NaSO4- 3.924e-009 3.665e-009 -8.406 -8.436 -0.030

KSO4- 1.954e-009 1.826e-009 -8.709 -8.739 -0.030

HSO4- 5.172e-012 4.831e-012 -11.286 -11.316 -0.030

CaHSO4+ 3.585e-014 3.349e-014 -13.445 -13.475 -0.030

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.97 -7.36 -4.39 CaSO4

Aragonite 1.30 -7.08 -8.38 CaCO3

Calcite 1.44 -7.08 -8.52 CaCO3

CO2(g) -4.18 -5.71 -1.53 CO2

Dolomite 2.84 -14.38 -17.22 CaMg(CO3)2

Gypsum -2.78 -7.36 -4.58 CaSO4:2H2O

H2(g) -26.48 -29.65 -3.17 H2

H2O(g) -1.36 -0.00 1.36 H2O

Halite -10.90 -9.30 1.59 NaCl

O2(g) -0.24 -3.17 -2.93 O2

Initial solution 118. 30/8/2012 17:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.505e-003 2.505e-003

Ca 9.164e-004 9.164e-004

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.197e-003 1.197e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.520

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 265

Density (g/cm3) = 0.99566

Activity of water = 1.000

Ionic strength = 3.703e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 1.886e-003

Total CO2 (mol/kg) = 1.886e-003

Temperature (deg C) = 30.560

Electrical balance (eq) = 9.014e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 2.03

Iterations = 6

Total H = 1.110138e+002

Total O = 5.551359e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 10.7422 0.6473

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 5.335e-005 4.988e-005 -4.273 -4.302 -0.029

H+ 3.210e-010 3.020e-010 -9.493 -9.520 -0.027

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 1.886e-003

HCO3- 1.311e-003 1.228e-003 -2.882 -2.911 -0.028

CO3-2 2.746e-004 2.117e-004 -3.561 -3.674 -0.113

CaCO3 2.121e-004 2.123e-004 -3.673 -3.673 0.000

MgCO3 7.250e-005 7.257e-005 -4.140 -4.139 0.000

CaHCO3+ 9.531e-006 8.931e-006 -5.021 -5.049 -0.028

MgHCO3+ 5.210e-006 4.874e-006 -5.283 -5.312 -0.029

CO2 7.849e-007 7.856e-007 -6.105 -6.105 0.000

NaCO3- 5.165e-008 4.832e-008 -7.287 -7.316 -0.029

NaHCO3 6.424e-009 6.430e-009 -8.192 -8.192 0.000

Ca 9.164e-004

Ca+2 6.859e-004 5.285e-004 -3.164 -3.277 -0.113

CaCO3 2.121e-004 2.123e-004 -3.673 -3.673 0.000

CaHCO3+ 9.531e-006 8.931e-006 -5.021 -5.049 -0.028

CaSO4 8.529e-006 8.536e-006 -5.069 -5.069 0.000

CaOH+ 3.104e-007 2.904e-007 -6.508 -6.537 -0.029

CaHSO4+ 1.736e-014 1.625e-014 -13.760 -13.789 -0.029

Cl 5.727e-005

Cl- 5.727e-005 5.355e-005 -4.242 -4.271 -0.029

H(0) 1.222e-030

H2 6.110e-031 6.115e-031 -30.214 -30.214 0.000

K 3.325e-006

K+ 3.323e-006 3.107e-006 -5.478 -5.508 -0.029

KSO4- 1.974e-009 1.847e-009 -8.705 -8.733 -0.029

KOH 3.564e-011 3.568e-011 -10.448 -10.448 0.000

Mg 5.184e-004

Mg+2 4.269e-004 3.298e-004 -3.370 -3.482 -0.112

MgCO3 7.250e-005 7.257e-005 -4.140 -4.139 0.000

MgOH+ 6.938e-006 6.491e-006 -5.159 -5.188 -0.029

MgSO4 6.839e-006 6.845e-006 -5.165 -5.165 0.000

MgHCO3+ 5.210e-006 4.874e-006 -5.283 -5.312 -0.029

Na 1.001e-005

Na+ 9.945e-006 9.309e-006 -5.002 -5.031 -0.029

NaCO3- 5.165e-008 4.832e-008 -7.287 -7.316 -0.029

NaHCO3 6.424e-009 6.430e-009 -8.192 -8.192 0.000

NaSO4- 3.971e-009 3.715e-009 -8.401 -8.430 -0.029

NaOH 2.035e-010 2.036e-010 -9.692 -9.691 0.000

O(0) 1.197e-003

O2 5.983e-004 5.988e-004 -3.223 -3.223 0.000

S(6) 1.154e-004

SO4-2 9.999e-005 7.692e-005 -4.000 -4.114 -0.114

CaSO4 8.529e-006 8.536e-006 -5.069 -5.069 0.000

MgSO4 6.839e-006 6.845e-006 -5.165 -5.165 0.000

NaSO4- 3.971e-009 3.715e-009 -8.401 -8.430 -0.029

KSO4- 1.974e-009 1.847e-009 -8.705 -8.733 -0.029

HSO4- 2.733e-012 2.557e-012 -11.563 -11.592 -0.029

CaHSO4+ 1.736e-014 1.625e-014 -13.760 -13.789 -0.029

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -3.00 -7.39 -4.39 CaSO4

Aragonite 1.42 -6.95 -8.37 CaCO3

Calcite 1.56 -6.95 -8.51 CaCO3

CO2(g) -4.57 -6.10 -1.53 CO2

Dolomite 3.11 -14.11 -17.22 CaMg(CO3)2

Gypsum -2.81 -7.39 -4.58 CaSO4:2H2O

H2(g) -27.04 -30.21 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.30 1.59 NaCl

O2(g) -0.29 -3.22 -2.93 O2

Initial solution 119. 30/8/2012 17:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.494e-003 2.494e-003

Ca 9.126e-004 9.126e-004

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.189e-003 1.189e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.620

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 261

Density (g/cm3) = 0.99573

Activity of water = 1.000

Ionic strength = 3.650e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 1.803e-003

Total CO2 (mol/kg) = 1.803e-003

Temperature (deg C) = 30.330

Electrical balance (eq) = 9.314e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 2.16

Iterations = 6

Total H = 1.110137e+002

Total O = 5.551335e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 10.6598 0.6419

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 6.604e-005 6.177e-005 -4.180 -4.209 -0.029

H+ 2.549e-010 2.399e-010 -9.594 -9.620 -0.026

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 1.803e-003

HCO3- 1.172e-003 1.099e-003 -2.931 -2.959 -0.028

CO3-2 3.074e-004 2.374e-004 -3.512 -3.624 -0.112

CaCO3 2.301e-004 2.303e-004 -3.638 -3.638 0.000

MgCO3 7.968e-005 7.975e-005 -4.099 -4.098 0.000

CaHCO3+ 8.262e-006 7.746e-006 -5.083 -5.111 -0.028

MgHCO3+ 4.575e-006 4.282e-006 -5.340 -5.368 -0.029

CO2 5.589e-007 5.594e-007 -6.253 -6.252 0.000

NaCO3- 5.726e-008 5.359e-008 -7.242 -7.271 -0.029

NaHCO3 5.747e-009 5.752e-009 -8.241 -8.240 0.000

Ca 9.126e-004

Ca+2 6.656e-004 5.138e-004 -3.177 -3.289 -0.112

CaCO3 2.301e-004 2.303e-004 -3.638 -3.638 0.000

CaSO4 8.317e-006 8.324e-006 -5.080 -5.080 0.000

CaHCO3+ 8.262e-006 7.746e-006 -5.083 -5.111 -0.028

CaOH+ 3.798e-007 3.555e-007 -6.420 -6.449 -0.029

CaHSO4+ 1.340e-014 1.254e-014 -13.873 -13.902 -0.029

Cl 5.727e-005

Cl- 5.727e-005 5.358e-005 -4.242 -4.271 -0.029

H(0) 7.727e-031

H2 3.864e-031 3.867e-031 -30.413 -30.413 0.000

K 3.325e-006

K+ 3.323e-006 3.109e-006 -5.478 -5.507 -0.029

KSO4- 1.977e-009 1.850e-009 -8.704 -8.733 -0.029

KOH 4.490e-011 4.493e-011 -10.348 -10.347 0.000

Mg 5.184e-004

Mg+2 4.190e-004 3.243e-004 -3.378 -3.489 -0.111

MgCO3 7.968e-005 7.975e-005 -4.099 -4.098 0.000

MgOH+ 8.414e-006 7.876e-006 -5.075 -5.104 -0.029

MgSO4 6.721e-006 6.726e-006 -5.173 -5.172 0.000

MgHCO3+ 4.575e-006 4.282e-006 -5.340 -5.368 -0.029

Na 1.001e-005

Na+ 9.940e-006 9.308e-006 -5.003 -5.031 -0.028

NaCO3- 5.726e-008 5.359e-008 -7.242 -7.271 -0.029

NaHCO3 5.747e-009 5.752e-009 -8.241 -8.240 0.000

NaSO4- 3.984e-009 3.729e-009 -8.400 -8.428 -0.029

NaOH 2.561e-010 2.564e-010 -9.592 -9.591 0.000

O(0) 1.189e-003

O2 5.945e-004 5.950e-004 -3.226 -3.225 0.000

S(6) 1.154e-004

SO4-2 1.003e-004 7.731e-005 -3.999 -4.112 -0.113

CaSO4 8.317e-006 8.324e-006 -5.080 -5.080 0.000

MgSO4 6.721e-006 6.726e-006 -5.173 -5.172 0.000

NaSO4- 3.984e-009 3.729e-009 -8.400 -8.428 -0.029

KSO4- 1.977e-009 1.850e-009 -8.704 -8.733 -0.029

HSO4- 2.169e-012 2.031e-012 -11.664 -11.692 -0.029

CaHSO4+ 1.340e-014 1.254e-014 -13.873 -13.902 -0.029

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -3.01 -7.40 -4.39 CaSO4

Aragonite 1.46 -6.91 -8.37 CaCO3

Calcite 1.60 -6.91 -8.51 CaCO3

CO2(g) -4.72 -6.25 -1.53 CO2

Dolomite 3.18 -14.03 -17.21 CaMg(CO3)2

Gypsum -2.82 -7.40 -4.58 CaSO4:2H2O

H2(g) -27.24 -30.41 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.30 1.59 NaCl

O2(g) -0.30 -3.23 -2.93 O2

Initial solution 120. 30/8/2012 17:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.494e-003 2.494e-003

Ca 9.126e-004 9.126e-004

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 1.188e-003 1.188e-003

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 9.540

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 262

Density (g/cm3) = 0.99579

Activity of water = 1.000

Ionic strength = 3.692e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 1.867e-003

Total CO2 (mol/kg) = 1.867e-003

Temperature (deg C) = 30.130

Electrical balance (eq) = 9.314e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 2.11

Iterations = 6

Total H = 1.110138e+002

Total O = 5.551353e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 10.7558 0.6472

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 5.416e-005 5.064e-005 -4.266 -4.295 -0.029

H+ 3.065e-010 2.884e-010 -9.514 -9.540 -0.026

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 1.867e-003

HCO3- 1.286e-003 1.205e-003 -2.891 -2.919 -0.028

CO3-2 2.798e-004 2.159e-004 -3.553 -3.666 -0.113

CaCO3 2.129e-004 2.131e-004 -3.672 -3.671 0.000

MgCO3 7.336e-005 7.343e-005 -4.135 -4.134 0.000

CaHCO3+ 9.250e-006 8.669e-006 -5.034 -5.062 -0.028

MgHCO3+ 5.093e-006 4.766e-006 -5.293 -5.322 -0.029

CO2 7.385e-007 7.391e-007 -6.132 -6.131 0.000

NaCO3- 5.158e-008 4.826e-008 -7.288 -7.316 -0.029

NaHCO3 6.305e-009 6.310e-009 -8.200 -8.200 0.000

Ca 9.126e-004

Ca+2 6.817e-004 5.256e-004 -3.166 -3.279 -0.113

CaCO3 2.129e-004 2.131e-004 -3.672 -3.671 0.000

CaHCO3+ 9.250e-006 8.669e-006 -5.034 -5.062 -0.028

CaSO4 8.464e-006 8.471e-006 -5.072 -5.072 0.000

CaOH+ 3.232e-007 3.024e-007 -6.491 -6.519 -0.029

CaHSO4+ 1.636e-014 1.531e-014 -13.786 -13.815 -0.029

Cl 5.727e-005

Cl- 5.727e-005 5.356e-005 -4.242 -4.271 -0.029

H(0) 1.119e-030

H2 5.595e-031 5.600e-031 -30.252 -30.252 0.000

K 3.325e-006

K+ 3.323e-006 3.108e-006 -5.478 -5.508 -0.029

KSO4- 1.964e-009 1.838e-009 -8.707 -8.736 -0.029

KOH 3.733e-011 3.736e-011 -10.428 -10.428 0.000

Mg 5.184e-004

Mg+2 4.262e-004 3.295e-004 -3.370 -3.482 -0.112

MgCO3 7.336e-005 7.343e-005 -4.135 -4.134 0.000

MgOH+ 6.989e-006 6.540e-006 -5.156 -5.184 -0.029

MgSO4 6.772e-006 6.777e-006 -5.169 -5.169 0.000

MgHCO3+ 5.093e-006 4.766e-006 -5.293 -5.322 -0.029

Na 1.001e-005

Na+ 9.945e-006 9.310e-006 -5.002 -5.031 -0.029

NaCO3- 5.158e-008 4.826e-008 -7.288 -7.316 -0.029

NaHCO3 6.305e-009 6.310e-009 -8.200 -8.200 0.000

NaSO4- 3.968e-009 3.713e-009 -8.401 -8.430 -0.029

NaOH 2.131e-010 2.133e-010 -9.671 -9.671 0.000

O(0) 1.188e-003

O2 5.942e-004 5.947e-004 -3.226 -3.226 0.000

S(6) 1.154e-004

SO4-2 1.001e-004 7.706e-005 -3.999 -4.113 -0.114

CaSO4 8.464e-006 8.471e-006 -5.072 -5.072 0.000

MgSO4 6.772e-006 6.777e-006 -5.169 -5.169 0.000

NaSO4- 3.968e-009 3.713e-009 -8.401 -8.430 -0.029

KSO4- 1.964e-009 1.838e-009 -8.707 -8.736 -0.029

HSO4- 2.589e-012 2.422e-012 -11.587 -11.616 -0.029

CaHSO4+ 1.636e-014 1.531e-014 -13.786 -13.815 -0.029

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -3.01 -7.39 -4.39 CaSO4

Aragonite 1.43 -6.95 -8.37 CaCO3

Calcite 1.57 -6.95 -8.51 CaCO3

CO2(g) -4.61 -6.13 -1.53 CO2

Dolomite 3.11 -14.09 -17.21 CaMg(CO3)2

Gypsum -2.81 -7.39 -4.58 CaSO4:2H2O

H2(g) -27.08 -30.25 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.30 1.59 NaCl

O2(g) -0.30 -3.23 -2.93 O2

------------------

End of simulation.

------------------

------------------------------------

Reading input data for simulation 2.

------------------------------------

-----------

End of run.

-----------

Input file: C:\Users\huan\Desktop\Maolan downstream.pqi

Output file: C:\Users\huan\Desktop\Maolan downstream.pqo

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

------------------

Reading data base.

------------------

SOLUTION\_MASTER\_SPECIES

SOLUTION\_SPECIES

PHASES

EXCHANGE\_MASTER\_SPECIES

EXCHANGE\_SPECIES

SURFACE\_MASTER\_SPECIES

SURFACE\_SPECIES

RATES

END

------------------------------------

Reading input data for simulation 1.

------------------------------------

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

SOLUTION\_SPREAD

units mg/l

Description Number pH Temp O(0) Ca K Mg Na S(6) Cl Alkalinity

mg/L mg/L mg/L mg/L mg/L mg/L mg/L mg/L as HCO3

29/8/2012 11:54:20 1 8.28 28.6 11.05 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

29/8/2012 12:09:20 2 8.29 29 8.77 44.37 0.13 12.60 0.23 11.07999992 2.029999971 184.92

29/8/2012 12:24:20 3 8.28 28.9 9.36 43.47 0.13 12.60 0.23 11.07999992 2.029999971 181.14

29/8/2012 12:39:20 4 8.29 29.7 11.09 43.77 0.13 12.60 0.23 11.07999992 2.029999971 182.41

29/8/2012 12:54:20 5 8.32 29.5 8.9 41.22 0.13 12.60 0.23 11.07999992 2.029999971 171.69

29/8/2012 13:09:20 6 8.29 30.1 9.49 44.37 0.13 12.60 0.23 11.07999992 2.029999971 184.92

29/8/2012 13:24:20 7 8.31 30.3 9.41 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

29/8/2012 13:39:20 8 8.31 30 9.85 42.27 0.13 12.60 0.23 11.07999992 2.029999971 176.11

29/8/2012 13:54:20 9 8.34 29.9 10.47 42.57 0.13 12.60 0.23 11.07999992 2.029999971 177.36

29/8/2012 14:09:20 10 8.37 30 8.56 42.57 0.13 12.60 0.23 11.07999992 2.029999971 177.36

29/8/2012 14:24:20 11 8.32 30.1 9.3 43.17 0.13 12.60 0.23 11.07999992 2.029999971 179.88

29/8/2012 14:39:20 12 8.36 30.2 8.62 43.02 0.13 12.60 0.23 11.07999992 2.029999971 179.25

29/8/2012 14:54:20 13 8.34 30.2 9.72 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

29/8/2012 15:09:20 14 8.34 30.3 8.54 44.22 0.13 12.60 0.23 11.07999992 2.029999971 184.3

29/8/2012 15:24:20 15 8.31 30.3 8.91 44.22 0.13 12.60 0.23 11.07999992 2.029999971 184.3

29/8/2012 15:39:20 16 8.36 30.2 8.7 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

29/8/2012 15:54:20 17 8.38 30.1 8.17 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

29/8/2012 16:09:20 18 8.38 30.1 8.05 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

29/8/2012 16:24:20 19 8.39 30.1 7.83 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

29/8/2012 16:39:20 20 8.39 30 8.38 43.77 0.13 12.60 0.23 11.07999992 2.029999971 182.41

29/8/2012 16:54:20 21 8.4 30 8.13 43.47 0.13 12.60 0.23 11.07999992 2.029999971 181.14

29/8/2012 17:09:20 22 8.42 29.9 7.64 43.62 0.13 12.60 0.23 11.07999992 2.029999971 181.77

29/8/2012 17:24:20 23 8.42 29.9 8.02 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

29/8/2012 17:39:20 24 8.42 29.9 7.56 43.47 0.13 12.60 0.23 11.07999992 2.029999971 181.14

29/8/2012 17:54:20 25 8.42 29.8 7.65 43.47 0.13 12.60 0.23 11.07999992 2.029999971 181.14

29/8/2012 18:09:20 26 8.42 29.8 7.33 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

29/8/2012 18:24:20 27 8.43 29.7 7.38 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

29/8/2012 18:39:20 28 8.4 29.6 8.12 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

29/8/2012 18:54:20 29 8.42 29.5 7.78 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

29/8/2012 19:09:20 30 8.42 29.4 7.85 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

29/8/2012 19:24:20 31 8.42 29.3 7.78 43.17 0.13 12.60 0.23 11.07999992 2.029999971 179.88

29/8/2012 19:39:20 32 8.4 29.2 7.56 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

29/8/2012 19:54:20 33 8.4 29.2 7.66 43.17 0.13 12.60 0.23 11.07999992 2.029999971 179.88

29/8/2012 20:09:20 34 8.39 29.1 7.39 43.77 0.13 12.60 0.23 11.07999992 2.029999971 182.41

29/8/2012 20:24:20 35 8.38 29 7.93 43.62 0.13 12.60 0.23 11.07999992 2.029999971 181.77

29/8/2012 20:39:20 36 8.39 28.9 8.28 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

29/8/2012 20:54:20 37 8.36 28.8 7.3 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

29/8/2012 21:09:20 38 8.37 28.8 7.2 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

29/8/2012 21:24:20 39 8.36 28.7 7.49 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

29/8/2012 21:39:20 40 8.35 28.6 7.17 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

29/8/2012 21:54:20 41 8.34 28.5 7.67 43.77 0.13 12.60 0.23 11.07999992 2.029999971 182.41

29/8/2012 22:09:20 42 8.34 28.5 6.95 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

29/8/2012 22:24:20 43 8.32 28.4 6.97 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

29/8/2012 22:39:20 44 8.32 28.4 7.6 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

29/8/2012 22:54:20 45 8.32 28.3 7.24 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

29/8/2012 23:09:20 46 8.29 28.2 7.11 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

29/8/2012 23:24:20 47 8.31 28.2 7.28 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

29/8/2012 23:39:20 48 8.29 28.1 7.6 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

29/8/2012 23:54:20 49 8.3 28.1 7.16 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 00:09:20 50 8.3 28 7.6 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

30/8/2012 00:24:20 51 8.3 28 7.9 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

30/8/2012 00:39:20 52 8.29 27.9 7.52 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

30/8/2012 00:54:20 53 8.28 27.9 8.46 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 01:09:20 54 8.28 27.8 8.56 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 01:24:20 55 8.27 27.8 8.8 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 01:39:20 56 8.27 27.7 8.69 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 01:54:20 57 8.26 27.7 8.71 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 02:09:20 58 8.27 27.7 8.59 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

30/8/2012 02:24:20 59 8.26 27.6 8.52 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 02:39:20 60 8.25 27.6 8.58 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 02:54:20 61 8.22 27.5 8.41 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 03:09:20 62 8.22 27.5 8.29 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

30/8/2012 03:24:20 63 8.23 27.4 8.21 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 03:39:20 64 8.21 27.4 8.24 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 03:54:20 65 8.2 27.4 8.2 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 04:09:20 66 8.23 27.3 8.46 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 04:24:20 67 8.19 27.3 8.35 43.62 0.13 12.60 0.23 11.07999992 2.029999971 181.77

30/8/2012 04:39:20 68 8.18 27.2 8.45 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 04:54:20 69 8.17 27.1 8.2 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

30/8/2012 05:09:20 70 8.14 27.1 8.12 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 05:24:20 71 8.16 27.1 8.07 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 05:39:20 72 8.16 27 8.21 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 05:54:20 73 8.15 27 7.89 44.22 0.13 12.60 0.23 11.07999992 2.029999971 184.3

30/8/2012 06:09:20 74 8.14 27 7.98 44.22 0.13 12.60 0.23 11.07999992 2.029999971 184.3

30/8/2012 06:24:20 75 8.15 26.9 7.95 44.22 0.13 12.60 0.23 11.07999992 2.029999971 184.3

30/8/2012 06:39:20 76 8.15 26.9 7.99 44.22 0.13 12.60 0.23 11.07999992 2.029999971 184.3

30/8/2012 06:54:20 77 8.14 26.8 7.88 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 07:09:20 78 8.14 26.8 7.87 44.22 0.13 12.60 0.23 11.07999992 2.029999971 184.3

30/8/2012 07:24:20 79 8.15 26.7 7.85 44.22 0.13 12.60 0.23 11.07999992 2.029999971 184.3

30/8/2012 07:39:20 80 8.15 26.7 8.31 44.22 0.13 12.60 0.23 11.07999992 2.029999971 184.3

30/8/2012 07:54:20 81 8.16 26.7 8.06 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 08:09:20 82 8.16 26.7 8.18 43.17 0.13 12.60 0.23 11.07999992 2.029999971 179.88

30/8/2012 08:24:20 83 8.13 26.8 8.45 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

30/8/2012 08:39:20 84 8.15 26.8 8.42 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

30/8/2012 08:54:20 85 8.15 26.8 7.95 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

30/8/2012 09:09:20 86 8.16 26.9 8.45 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

30/8/2012 09:24:20 87 8.16 26.9 8.31 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

30/8/2012 09:39:20 88 8.18 26.9 7.03 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

30/8/2012 09:54:20 89 8.17 26.9 8.24 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 10:09:20 90 8.17 27 8.55 44.07 0.13 12.60 0.23 11.07999992 2.029999971 183.66

30/8/2012 10:24:20 91 8.12 27.1 8.27 44.22 0.13 12.60 0.23 11.07999992 2.029999971 184.3

30/8/2012 10:39:20 92 8.18 27.2 8.57 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

30/8/2012 10:54:20 93 8.22 27.5 8.46 43.92 0.13 12.60 0.23 11.07999992 2.029999971 183.03

30/8/2012 11:09:20 94 8.22 27.7 8.81 43.62 0.13 12.60 0.23 11.07999992 2.029999971 181.77

30/8/2012 11:24:20 95 8.22 27.8 8.94 43.62 0.13 12.60 0.23 11.07999992 2.029999971 181.77

30/8/2012 11:39:20 96 8.2 27.7 9.08 43.62 0.13 12.60 0.23 11.07999992 2.029999971 181.77

30/8/2012 11:54:20 97 8.2 27.9 9.04 43.77 0.13 12.60 0.23 11.07999992 2.029999971 182.41

30/8/2012 12:09:20 98 8.24 28.2 9.31 43.77 0.13 12.60 0.23 11.07999992 2.029999971 182.41

30/8/2012 12:24:20 99 8.27 28.4 9.82 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

30/8/2012 12:39:20 100 8.3 28.7 9.34 43.62 0.13 12.60 0.23 11.07999992 2.029999971 181.77

30/8/2012 12:54:20 101 8.33 29 9.94 43.62 0.13 12.60 0.23 11.07999992 2.029999971 181.77

30/8/2012 13:09:20 102 8.31 29.3 10.25 43.02 0.13 12.60 0.23 11.07999992 2.029999971 179.25

30/8/2012 13:24:20 103 8.34 29.7 10.64 43.62 0.13 12.60 0.23 11.07999992 2.029999971 181.77

30/8/2012 13:39:20 104 8.35 29.8 10.63 43.02 0.13 12.60 0.23 11.07999992 2.029999971 179.25

30/8/2012 13:54:20 105 8.34 29.9 9.28 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

30/8/2012 14:09:20 106 8.38 30.1 10.57 43.77 0.13 12.60 0.23 11.07999992 2.029999971 182.41

30/8/2012 14:24:20 107 8.39 30.2 10.24 42.42 0.13 12.60 0.23 11.07999992 2.029999971 176.74

30/8/2012 14:54:20 108 8.38 30.4 11.46 42.87 0.13 12.60 0.23 11.07999992 2.029999971 178.63

30/8/2012 15:09:20 109 8.39 30.5 9.94 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

30/8/2012 15:24:20 110 8.37 30.4 10.54 43.17 0.13 12.60 0.23 11.07999992 2.029999971 179.88

30/8/2012 15:39:20 111 8.39 30.4 9.8 42.87 0.13 12.60 0.23 11.07999992 2.029999971 178.63

30/8/2012 15:54:20 112 8.39 30.4 9.32 43.47 0.13 12.60 0.23 11.07999992 2.029999971 181.14

30/8/2012 16:09:20 113 8.38 30.4 9.31 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

30/8/2012 16:24:20 114 8.4 30.4 9.28 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

30/8/2012 16:39:20 115 8.39 30.4 7.52 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

30/8/2012 16:54:20 116 8.38 30.3 7.89 43.17 0.13 12.60 0.23 11.07999992 2.029999971 179.88

30/8/2012 17:09:20 117 8.38 30.3 7.5 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

30/8/2012 17:24:20 118 8.39 30.3 7.72 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

30/8/2012 17:39:20 119 8.38 30.2 7.49 43.17 0.13 12.60 0.23 11.07999992 2.029999971 179.88

30/8/2012 17:54:20 120 8.42 30.2 8.01 43.32 0.13 12.60 0.23 11.07999992 2.029999971 180.52

SELECTED\_OUTPUT

file C:\Users\huan\Desktop\selected output downstream.sel

reset false

saturation\_indices Calcite CO2(g)

-------------------------------------------

Beginning of initial solution calculations.

-------------------------------------------

Initial solution 1. 29/8/2012 11:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.908e-004 6.908e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.280

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 318

Density (g/cm3) = 0.99627

Activity of water = 1.000

Ionic strength = 4.695e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.910e-003

Total CO2 (mol/kg) = 2.910e-003

Temperature (deg C) = 28.600

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551607e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.0800 0.7232

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.686e-006 2.492e-006 -5.571 -5.604 -0.033

H+ 5.613e-009 5.248e-009 -8.251 -8.280 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.910e-003

HCO3- 2.765e-003 2.572e-003 -2.558 -2.590 -0.031

CaCO3 3.370e-005 3.374e-005 -4.472 -4.472 0.000

CO3-2 3.287e-005 2.463e-005 -4.483 -4.608 -0.125

CO2 2.911e-005 2.914e-005 -4.536 -4.535 0.000

CaHCO3+ 2.802e-005 2.607e-005 -4.552 -4.584 -0.031

MgHCO3+ 1.214e-005 1.127e-005 -4.916 -4.948 -0.032

MgCO3 9.136e-006 9.146e-006 -5.039 -5.039 0.000

NaHCO3 1.341e-008 1.342e-008 -7.873 -7.872 0.000

NaCO3- 5.483e-009 5.092e-009 -8.261 -8.293 -0.032

Ca 1.081e-003

Ca+2 1.008e-003 7.551e-004 -2.997 -3.122 -0.125

CaCO3 3.370e-005 3.374e-005 -4.472 -4.472 0.000

CaHCO3+ 2.802e-005 2.607e-005 -4.552 -4.584 -0.031

CaSO4 1.130e-005 1.132e-005 -4.947 -4.946 0.000

CaOH+ 2.571e-008 2.388e-008 -7.590 -7.622 -0.032

CaHSO4+ 3.924e-013 3.644e-013 -12.406 -12.438 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.275 -0.032

H(0) 3.760e-028

H2 1.880e-028 1.882e-028 -27.726 -27.725 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.804e-009 1.675e-009 -8.744 -8.776 -0.032

KOH 2.035e-012 2.038e-012 -11.691 -11.691 0.000

Mg 5.184e-004

Mg+2 4.899e-004 3.682e-004 -3.310 -3.434 -0.124

MgHCO3+ 1.214e-005 1.127e-005 -4.916 -4.948 -0.032

MgCO3 9.136e-006 9.146e-006 -5.039 -5.039 0.000

MgSO4 6.864e-006 6.872e-006 -5.163 -5.163 0.000

MgOH+ 3.781e-007 3.512e-007 -6.422 -6.454 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.278e-006 -5.001 -5.033 -0.032

NaHCO3 1.341e-008 1.342e-008 -7.873 -7.872 0.000

NaCO3- 5.483e-009 5.092e-009 -8.261 -8.293 -0.032

NaSO4- 3.721e-009 3.455e-009 -8.429 -8.462 -0.032

NaOH 1.167e-011 1.168e-011 -10.933 -10.933 0.000

O(0) 6.908e-004

O2 3.454e-004 3.458e-004 -3.462 -3.461 0.000

S(6) 1.154e-004

SO4-2 9.720e-005 7.265e-005 -4.012 -4.139 -0.126

CaSO4 1.130e-005 1.132e-005 -4.947 -4.946 0.000

MgSO4 6.864e-006 6.872e-006 -5.163 -5.163 0.000

NaSO4- 3.721e-009 3.455e-009 -8.429 -8.462 -0.032

KSO4- 1.804e-009 1.675e-009 -8.744 -8.776 -0.032

HSO4- 4.323e-011 4.014e-011 -10.364 -10.396 -0.032

CaHSO4+ 3.924e-013 3.644e-013 -12.406 -12.438 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.63 -7.73 -8.36 CaCO3

Calcite 0.77 -7.73 -8.50 CaCO3

CO2(g) -3.03 -4.54 -1.51 CO2

Dolomite 1.40 -15.77 -17.17 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.56 -27.73 -3.17 H2

H2O(g) -1.42 -0.00 1.42 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.54 -3.46 -2.92 O2

Initial solution 2. 29/8/2012 12:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.031e-003 3.031e-003

Ca 1.107e-003 1.107e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.483e-004 5.483e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.290

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 327

Density (g/cm3) = 0.99616

Activity of water = 1.000

Ionic strength = 4.772e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.976e-003

Total CO2 (mol/kg) = 2.976e-003

Temperature (deg C) = 29.000

Electrical balance (eq) = -5.455e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.87

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551613e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.0126 0.7202

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.831e-006 2.625e-006 -5.548 -5.581 -0.033

H+ 5.488e-009 5.129e-009 -8.261 -8.290 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.976e-003

HCO3- 2.825e-003 2.627e-003 -2.549 -2.581 -0.032

CaCO3 3.649e-005 3.653e-005 -4.438 -4.437 0.000

CO3-2 3.467e-005 2.593e-005 -4.460 -4.586 -0.126

CaHCO3+ 2.934e-005 2.728e-005 -4.533 -4.564 -0.032

CO2 2.893e-005 2.896e-005 -4.539 -4.538 0.000

MgHCO3+ 1.238e-005 1.149e-005 -4.907 -4.940 -0.032

MgCO3 9.639e-006 9.650e-006 -5.016 -5.015 0.000

NaHCO3 1.368e-008 1.370e-008 -7.864 -7.863 0.000

NaCO3- 5.886e-009 5.463e-009 -8.230 -8.263 -0.032

Ca 1.107e-003

Ca+2 1.030e-003 7.698e-004 -2.987 -3.114 -0.126

CaCO3 3.649e-005 3.653e-005 -4.438 -4.437 0.000

CaHCO3+ 2.934e-005 2.728e-005 -4.533 -4.564 -0.032

CaSO4 1.151e-005 1.152e-005 -4.939 -4.938 0.000

CaOH+ 2.684e-008 2.491e-008 -7.571 -7.604 -0.032

CaHSO4+ 3.929e-013 3.647e-013 -12.406 -12.438 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.311e-005 -4.242 -4.275 -0.033

H(0) 3.577e-028

H2 1.788e-028 1.790e-028 -27.748 -27.747 0.000

K 3.326e-006

K+ 3.324e-006 3.082e-006 -5.478 -5.511 -0.033

KSO4- 1.808e-009 1.678e-009 -8.743 -8.775 -0.032

KOH 2.081e-012 2.084e-012 -11.682 -11.681 0.000

Mg 5.184e-004

Mg+2 4.891e-004 3.668e-004 -3.311 -3.436 -0.125

MgHCO3+ 1.238e-005 1.149e-005 -4.907 -4.940 -0.032

MgCO3 9.639e-006 9.650e-006 -5.016 -5.015 0.000

MgSO4 6.875e-006 6.883e-006 -5.163 -5.162 0.000

MgOH+ 3.995e-007 3.708e-007 -6.398 -6.431 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.272e-006 -5.001 -5.033 -0.032

NaHCO3 1.368e-008 1.370e-008 -7.864 -7.863 0.000

NaCO3- 5.886e-009 5.463e-009 -8.230 -8.263 -0.032

NaSO4- 3.713e-009 3.446e-009 -8.430 -8.463 -0.032

NaOH 1.193e-011 1.194e-011 -10.923 -10.923 0.000

O(0) 5.483e-004

O2 2.741e-004 2.744e-004 -3.562 -3.562 0.000

S(6) 1.154e-004

SO4-2 9.698e-005 7.232e-005 -4.013 -4.141 -0.127

CaSO4 1.151e-005 1.152e-005 -4.939 -4.938 0.000

MgSO4 6.875e-006 6.883e-006 -5.163 -5.162 0.000

NaSO4- 3.713e-009 3.446e-009 -8.430 -8.463 -0.032

KSO4- 1.808e-009 1.678e-009 -8.743 -8.775 -0.032

HSO4- 4.245e-011 3.940e-011 -10.372 -10.404 -0.032

CaHSO4+ 3.929e-013 3.647e-013 -12.406 -12.438 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.87 -7.25 -4.38 CaSO4

Aragonite 0.66 -7.70 -8.36 CaCO3

Calcite 0.80 -7.70 -8.50 CaCO3

CO2(g) -3.02 -4.54 -1.51 CO2

Dolomite 1.46 -15.72 -17.18 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.58 -27.75 -3.17 H2

H2O(g) -1.41 -0.00 1.41 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.64 -3.56 -2.92 O2

Initial solution 3. 29/8/2012 12:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.969e-003 2.969e-003

Ca 1.085e-003 1.085e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.852e-004 5.852e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.280

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 321

Density (g/cm3) = 0.99619

Activity of water = 1.000

Ionic strength = 4.705e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.919e-003

Total CO2 (mol/kg) = 2.919e-003

Temperature (deg C) = 28.900

Electrical balance (eq) = -3.751e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.61

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551599e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.0378 0.7214

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.745e-006 2.547e-006 -5.561 -5.594 -0.033

H+ 5.614e-009 5.248e-009 -8.251 -8.280 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.919e-003

HCO3- 2.772e-003 2.579e-003 -2.557 -2.589 -0.031

CaCO3 3.429e-005 3.433e-005 -4.465 -4.464 0.000

CO3-2 3.315e-005 2.484e-005 -4.480 -4.605 -0.125

CO2 2.910e-005 2.913e-005 -4.536 -4.536 0.000

CaHCO3+ 2.828e-005 2.631e-005 -4.549 -4.580 -0.031

MgHCO3+ 1.218e-005 1.131e-005 -4.914 -4.946 -0.032

MgCO3 9.246e-006 9.256e-006 -5.034 -5.034 0.000

NaHCO3 1.344e-008 1.346e-008 -7.872 -7.871 0.000

NaCO3- 5.610e-009 5.210e-009 -8.251 -8.283 -0.032

Ca 1.085e-003

Ca+2 1.011e-003 7.570e-004 -2.995 -3.121 -0.126

CaCO3 3.429e-005 3.433e-005 -4.465 -4.464 0.000

CaHCO3+ 2.828e-005 2.631e-005 -4.549 -4.580 -0.031

CaSO4 1.135e-005 1.136e-005 -4.945 -4.945 0.000

CaOH+ 2.578e-008 2.393e-008 -7.589 -7.621 -0.032

CaHSO4+ 3.956e-013 3.673e-013 -12.403 -12.435 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 3.749e-028

H2 1.874e-028 1.877e-028 -27.727 -27.727 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.811e-009 1.681e-009 -8.742 -8.774 -0.032

KOH 2.035e-012 2.037e-012 -11.691 -11.691 0.000

Mg 5.184e-004

Mg+2 4.897e-004 3.679e-004 -3.310 -3.434 -0.124

MgHCO3+ 1.218e-005 1.131e-005 -4.914 -4.946 -0.032

MgCO3 9.246e-006 9.256e-006 -5.034 -5.034 0.000

MgSO4 6.902e-006 6.909e-006 -5.161 -5.161 0.000

MgOH+ 3.880e-007 3.603e-007 -6.411 -6.443 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.344e-008 1.346e-008 -7.872 -7.871 0.000

NaCO3- 5.610e-009 5.210e-009 -8.251 -8.283 -0.032

NaSO4- 3.723e-009 3.457e-009 -8.429 -8.461 -0.032

NaOH 1.167e-011 1.168e-011 -10.933 -10.933 0.000

O(0) 5.852e-004

O2 2.926e-004 2.929e-004 -3.534 -3.533 0.000

S(6) 1.154e-004

SO4-2 9.712e-005 7.256e-005 -4.013 -4.139 -0.127

CaSO4 1.135e-005 1.136e-005 -4.945 -4.945 0.000

MgSO4 6.902e-006 6.909e-006 -5.161 -5.161 0.000

NaSO4- 3.723e-009 3.457e-009 -8.429 -8.461 -0.032

KSO4- 1.811e-009 1.681e-009 -8.742 -8.774 -0.032

HSO4- 4.347e-011 4.036e-011 -10.362 -10.394 -0.032

CaHSO4+ 3.956e-013 3.673e-013 -12.403 -12.435 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.64 -7.73 -8.36 CaCO3

Calcite 0.78 -7.73 -8.50 CaCO3

CO2(g) -3.02 -4.54 -1.51 CO2

Dolomite 1.41 -15.77 -17.18 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.56 -27.73 -3.17 H2

H2O(g) -1.41 -0.00 1.41 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.61 -3.53 -2.92 O2

Initial solution 4. 29/8/2012 12:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.990e-003 2.990e-003

Ca 1.092e-003 1.092e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.933e-004 6.933e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.290

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 328

Density (g/cm3) = 0.99595

Activity of water = 1.000

Ionic strength = 4.722e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.934e-003

Total CO2 (mol/kg) = 2.934e-003

Temperature (deg C) = 29.700

Electrical balance (eq) = -4.336e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.70

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551615e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9818 0.7200

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.977e-006 2.761e-006 -5.526 -5.559 -0.033

H+ 5.487e-009 5.129e-009 -8.261 -8.290 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.934e-003

HCO3- 2.784e-003 2.590e-003 -2.555 -2.587 -0.031

CaCO3 3.654e-005 3.657e-005 -4.437 -4.437 0.000

CO3-2 3.458e-005 2.588e-005 -4.461 -4.587 -0.126

CaHCO3+ 2.879e-005 2.678e-005 -4.541 -4.572 -0.031

CO2 2.833e-005 2.836e-005 -4.548 -4.547 0.000

MgHCO3+ 1.226e-005 1.138e-005 -4.912 -4.944 -0.032

MgCO3 9.734e-006 9.744e-006 -5.012 -5.011 0.000

NaHCO3 1.349e-008 1.351e-008 -7.870 -7.869 0.000

NaCO3- 6.081e-009 5.645e-009 -8.216 -8.248 -0.032

Ca 1.092e-003

Ca+2 1.016e-003 7.598e-004 -2.993 -3.119 -0.126

CaCO3 3.654e-005 3.657e-005 -4.437 -4.437 0.000

CaHCO3+ 2.879e-005 2.678e-005 -4.541 -4.572 -0.031

CaSO4 1.144e-005 1.145e-005 -4.942 -4.941 0.000

CaOH+ 2.648e-008 2.458e-008 -7.577 -7.609 -0.032

CaHSO4+ 3.940e-013 3.658e-013 -12.404 -12.437 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 3.553e-028

H2 1.776e-028 1.778e-028 -27.750 -27.750 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.830e-009 1.699e-009 -8.737 -8.770 -0.032

KOH 2.082e-012 2.084e-012 -11.682 -11.681 0.000

Mg 5.184e-004

Mg+2 4.890e-004 3.670e-004 -3.311 -3.435 -0.125

MgHCO3+ 1.226e-005 1.138e-005 -4.912 -4.944 -0.032

MgCO3 9.734e-006 9.744e-006 -5.012 -5.011 0.000

MgSO4 7.005e-006 7.013e-006 -5.155 -5.154 0.000

MgOH+ 4.250e-007 3.946e-007 -6.372 -6.404 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.349e-008 1.351e-008 -7.870 -7.869 0.000

NaCO3- 6.081e-009 5.645e-009 -8.216 -8.248 -0.032

NaSO4- 3.730e-009 3.463e-009 -8.428 -8.461 -0.032

NaOH 1.193e-011 1.195e-011 -10.923 -10.923 0.000

O(0) 6.933e-004

O2 3.467e-004 3.470e-004 -3.460 -3.460 0.000

S(6) 1.154e-004

SO4-2 9.692e-005 7.235e-005 -4.014 -4.141 -0.127

CaSO4 1.144e-005 1.145e-005 -4.942 -4.941 0.000

MgSO4 7.005e-006 7.013e-006 -5.155 -5.154 0.000

NaSO4- 3.730e-009 3.463e-009 -8.428 -8.461 -0.032

KSO4- 1.830e-009 1.699e-009 -8.737 -8.770 -0.032

HSO4- 4.314e-011 4.005e-011 -10.365 -10.397 -0.032

CaHSO4+ 3.940e-013 3.658e-013 -12.404 -12.437 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.66 -7.71 -8.37 CaCO3

Calcite 0.80 -7.71 -8.51 CaCO3

CO2(g) -3.03 -4.55 -1.52 CO2

Dolomite 1.47 -15.73 -17.20 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.58 -27.75 -3.17 H2

H2O(g) -1.39 -0.00 1.39 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.54 -3.46 -2.92 O2

Initial solution 5. 29/8/2012 12:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.814e-003 2.814e-003

Ca 1.029e-003 1.029e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.564e-004 5.564e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.320

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 312

Density (g/cm3) = 0.99600

Activity of water = 1.000

Ionic strength = 4.521e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.757e-003

Total CO2 (mol/kg) = 2.757e-003

Temperature (deg C) = 29.500

Electrical balance (eq) = 5.094e-006

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.09

Iterations = 8

Total H = 1.110151e+002

Total O = 5.551548e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9440 0.7172

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.140e-006 2.916e-006 -5.503 -5.535 -0.032

H+ 5.114e-009 4.786e-009 -8.291 -8.320 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.757e-003

HCO3- 2.616e-003 2.436e-003 -2.582 -2.613 -0.031

CaCO3 3.464e-005 3.468e-005 -4.460 -4.460 0.000

CO3-2 3.454e-005 2.600e-005 -4.462 -4.585 -0.123

CaHCO3+ 2.559e-005 2.383e-005 -4.592 -4.623 -0.031

CO2 2.492e-005 2.495e-005 -4.603 -4.603 0.000

MgHCO3+ 1.158e-005 1.077e-005 -4.936 -4.968 -0.032

MgCO3 9.812e-006 9.823e-006 -5.008 -5.008 0.000

NaHCO3 1.271e-008 1.273e-008 -7.896 -7.895 0.000

NaCO3- 6.049e-009 5.624e-009 -8.218 -8.250 -0.032

Ca 1.029e-003

Ca+2 9.575e-004 7.204e-004 -3.019 -3.142 -0.124

CaCO3 3.464e-005 3.468e-005 -4.460 -4.460 0.000

CaHCO3+ 2.559e-005 2.383e-005 -4.592 -4.623 -0.031

CaSO4 1.094e-005 1.095e-005 -4.961 -4.961 0.000

CaOH+ 2.687e-008 2.498e-008 -7.571 -7.602 -0.032

CaHSO4+ 3.501e-013 3.255e-013 -12.456 -12.487 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.321e-005 -4.242 -4.274 -0.032

H(0) 3.100e-028

H2 1.550e-028 1.552e-028 -27.810 -27.809 0.000

K 3.325e-006

K+ 3.324e-006 3.088e-006 -5.478 -5.510 -0.032

KSO4- 1.843e-009 1.713e-009 -8.735 -8.766 -0.032

KOH 2.234e-012 2.237e-012 -11.651 -11.650 0.000

Mg 5.184e-004

Mg+2 4.895e-004 3.694e-004 -3.310 -3.432 -0.122

MgHCO3+ 1.158e-005 1.077e-005 -4.936 -4.968 -0.032

MgCO3 9.812e-006 9.823e-006 -5.008 -5.008 0.000

MgSO4 7.087e-006 7.095e-006 -5.150 -5.149 0.000

MgOH+ 4.498e-007 4.182e-007 -6.347 -6.379 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.289e-006 -5.001 -5.032 -0.031

NaHCO3 1.271e-008 1.273e-008 -7.896 -7.895 0.000

NaCO3- 6.049e-009 5.624e-009 -8.218 -8.250 -0.032

NaSO4- 3.764e-009 3.499e-009 -8.424 -8.456 -0.032

NaOH 1.281e-011 1.282e-011 -10.893 -10.892 0.000

O(0) 5.564e-004

O2 2.782e-004 2.785e-004 -3.556 -3.555 0.000

S(6) 1.154e-004

SO4-2 9.734e-005 7.308e-005 -4.012 -4.136 -0.124

CaSO4 1.094e-005 1.095e-005 -4.961 -4.961 0.000

MgSO4 7.087e-006 7.095e-006 -5.150 -5.149 0.000

NaSO4- 3.764e-009 3.499e-009 -8.424 -8.456 -0.032

KSO4- 1.843e-009 1.713e-009 -8.735 -8.766 -0.032

HSO4- 4.042e-011 3.758e-011 -10.393 -10.425 -0.032

CaHSO4+ 3.501e-013 3.255e-013 -12.456 -12.487 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.90 -7.28 -4.38 CaSO4

Aragonite 0.64 -7.73 -8.37 CaCO3

Calcite 0.78 -7.73 -8.51 CaCO3

CO2(g) -3.08 -4.60 -1.52 CO2

Dolomite 1.45 -15.74 -17.19 CaMg(CO3)2

Gypsum -2.70 -7.28 -4.58 CaSO4:2H2O

H2(g) -24.64 -27.81 -3.17 H2

H2O(g) -1.40 -0.00 1.40 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.63 -3.56 -2.92 O2

Initial solution 6. 29/8/2012 13:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.031e-003 3.031e-003

Ca 1.107e-003 1.107e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.933e-004 5.933e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.290

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 334

Density (g/cm3) = 0.99583

Activity of water = 1.000

Ionic strength = 4.765e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.973e-003

Total CO2 (mol/kg) = 2.973e-003

Temperature (deg C) = 30.100

Electrical balance (eq) = -5.455e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.88

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551617e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9328 0.7180

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.065e-006 2.842e-006 -5.514 -5.546 -0.033

H+ 5.488e-009 5.129e-009 -8.261 -8.290 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.973e-003

HCO3- 2.819e-003 2.621e-003 -2.550 -2.581 -0.032

CaCO3 3.801e-005 3.805e-005 -4.420 -4.420 0.000

CO3-2 3.530e-005 2.639e-005 -4.452 -4.579 -0.126

CaHCO3+ 2.962e-005 2.754e-005 -4.528 -4.560 -0.032

CO2 2.856e-005 2.860e-005 -4.544 -4.544 0.000

MgHCO3+ 1.241e-005 1.152e-005 -4.906 -4.939 -0.032

MgCO3 9.962e-006 9.973e-006 -5.002 -5.001 0.000

NaHCO3 1.365e-008 1.367e-008 -7.865 -7.864 0.000

NaCO3- 6.321e-009 5.866e-009 -8.199 -8.232 -0.032

Ca 1.107e-003

Ca+2 1.028e-003 7.681e-004 -2.988 -3.115 -0.127

CaCO3 3.801e-005 3.805e-005 -4.420 -4.420 0.000

CaHCO3+ 2.962e-005 2.754e-005 -4.528 -4.560 -0.032

CaSO4 1.157e-005 1.158e-005 -4.937 -4.936 0.000

CaOH+ 2.678e-008 2.485e-008 -7.572 -7.605 -0.032

CaHSO4+ 4.009e-013 3.720e-013 -12.397 -12.429 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.311e-005 -4.242 -4.275 -0.033

H(0) 3.539e-028

H2 1.769e-028 1.771e-028 -27.752 -27.752 0.000

K 3.326e-006

K+ 3.324e-006 3.082e-006 -5.478 -5.511 -0.033

KSO4- 1.837e-009 1.705e-009 -8.736 -8.768 -0.032

KOH 2.081e-012 2.084e-012 -11.682 -11.681 0.000

Mg 5.184e-004

Mg+2 4.885e-004 3.662e-004 -3.311 -3.436 -0.125

MgHCO3+ 1.241e-005 1.152e-005 -4.906 -4.939 -0.032

MgCO3 9.962e-006 9.973e-006 -5.002 -5.001 0.000

MgSO4 7.038e-006 7.045e-006 -5.153 -5.152 0.000

MgOH+ 4.393e-007 4.077e-007 -6.357 -6.390 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.271e-006 -5.001 -5.033 -0.032

NaHCO3 1.365e-008 1.367e-008 -7.865 -7.864 0.000

NaCO3- 6.321e-009 5.866e-009 -8.199 -8.232 -0.032

NaSO4- 3.728e-009 3.459e-009 -8.429 -8.461 -0.032

NaOH 1.193e-011 1.194e-011 -10.923 -10.923 0.000

O(0) 5.933e-004

O2 2.966e-004 2.970e-004 -3.528 -3.527 0.000

S(6) 1.154e-004

SO4-2 9.676e-005 7.212e-005 -4.014 -4.142 -0.128

CaSO4 1.157e-005 1.158e-005 -4.937 -4.936 0.000

MgSO4 7.038e-006 7.045e-006 -5.153 -5.152 0.000

NaSO4- 3.728e-009 3.459e-009 -8.429 -8.461 -0.032

KSO4- 1.837e-009 1.705e-009 -8.736 -8.768 -0.032

HSO4- 4.341e-011 4.029e-011 -10.362 -10.395 -0.032

CaHSO4+ 4.009e-013 3.720e-013 -12.397 -12.429 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.87 -7.26 -4.39 CaSO4

Aragonite 0.68 -7.69 -8.37 CaCO3

Calcite 0.82 -7.69 -8.51 CaCO3

CO2(g) -3.02 -4.54 -1.53 CO2

Dolomite 1.50 -15.71 -17.21 CaMg(CO3)2

Gypsum -2.67 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.58 -27.75 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.60 -3.53 -2.93 O2

Initial solution 7. 29/8/2012 13:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.883e-004 5.883e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.310

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 329

Density (g/cm3) = 0.99577

Activity of water = 1.000

Ionic strength = 4.679e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.897e-003

Total CO2 (mol/kg) = 2.897e-003

Temperature (deg C) = 30.300

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551594e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8959 0.7162

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.254e-006 3.019e-006 -5.488 -5.520 -0.033

H+ 5.239e-009 4.898e-009 -8.281 -8.310 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.897e-003

HCO3- 2.746e-003 2.555e-003 -2.561 -2.593 -0.031

CaCO3 3.824e-005 3.828e-005 -4.417 -4.417 0.000

CO3-2 3.607e-005 2.702e-005 -4.443 -4.568 -0.125

CaHCO3+ 2.828e-005 2.631e-005 -4.548 -4.580 -0.031

CO2 2.653e-005 2.656e-005 -4.576 -4.576 0.000

MgHCO3+ 1.213e-005 1.126e-005 -4.916 -4.948 -0.032

MgCO3 1.025e-005 1.026e-005 -4.989 -4.989 0.000

NaHCO3 1.331e-008 1.333e-008 -7.876 -7.875 0.000

NaCO3- 6.537e-009 6.070e-009 -8.185 -8.217 -0.032

Ca 1.081e-003

Ca+2 1.003e-003 7.512e-004 -2.999 -3.124 -0.126

CaCO3 3.824e-005 3.828e-005 -4.417 -4.417 0.000

CaHCO3+ 2.828e-005 2.631e-005 -4.548 -4.580 -0.031

CaSO4 1.138e-005 1.139e-005 -4.944 -4.944 0.000

CaOH+ 2.741e-008 2.545e-008 -7.562 -7.594 -0.032

CaHSO4+ 3.772e-013 3.503e-013 -12.423 -12.456 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 3.221e-028

H2 1.611e-028 1.612e-028 -27.793 -27.793 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.850e-009 1.717e-009 -8.733 -8.765 -0.032

KOH 2.181e-012 2.183e-012 -11.661 -11.661 0.000

Mg 5.184e-004

Mg+2 4.884e-004 3.669e-004 -3.311 -3.435 -0.124

MgHCO3+ 1.213e-005 1.126e-005 -4.916 -4.948 -0.032

MgCO3 1.025e-005 1.026e-005 -4.989 -4.989 0.000

MgSO4 7.112e-006 7.119e-006 -5.148 -5.148 0.000

MgOH+ 4.688e-007 4.353e-007 -6.329 -6.361 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.331e-008 1.333e-008 -7.876 -7.875 0.000

NaCO3- 6.537e-009 6.070e-009 -8.185 -8.217 -0.032

NaSO4- 3.745e-009 3.478e-009 -8.426 -8.459 -0.032

NaOH 1.250e-011 1.251e-011 -10.903 -10.903 0.000

O(0) 5.883e-004

O2 2.941e-004 2.945e-004 -3.531 -3.531 0.000

S(6) 1.154e-004

SO4-2 9.688e-005 7.238e-005 -4.014 -4.140 -0.127

CaSO4 1.138e-005 1.139e-005 -4.944 -4.944 0.000

MgSO4 7.112e-006 7.119e-006 -5.148 -5.148 0.000

NaSO4- 3.745e-009 3.478e-009 -8.426 -8.459 -0.032

KSO4- 1.850e-009 1.717e-009 -8.733 -8.765 -0.032

HSO4- 4.177e-011 3.878e-011 -10.379 -10.411 -0.032

CaHSO4+ 3.772e-013 3.503e-013 -12.423 -12.456 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.39 CaSO4

Aragonite 0.68 -7.69 -8.37 CaCO3

Calcite 0.82 -7.69 -8.51 CaCO3

CO2(g) -3.05 -4.58 -1.53 CO2

Dolomite 1.51 -15.70 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.62 -27.79 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.60 -3.53 -2.93 O2

Initial solution 8. 29/8/2012 13:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.887e-003 2.887e-003

Ca 1.055e-003 1.055e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.158e-004 6.158e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.310

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 321

Density (g/cm3) = 0.99585

Activity of water = 1.000

Ionic strength = 4.601e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.828e-003

Total CO2 (mol/kg) = 2.828e-003

Temperature (deg C) = 30.000

Electrical balance (eq) = -1.495e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.25

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551576e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9248 0.7173

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.183e-006 2.954e-006 -5.497 -5.530 -0.032

H+ 5.236e-009 4.898e-009 -8.281 -8.310 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.828e-003

HCO3- 2.682e-003 2.497e-003 -2.572 -2.603 -0.031

CaCO3 3.617e-005 3.621e-005 -4.442 -4.441 0.000

CO3-2 3.499e-005 2.627e-005 -4.456 -4.581 -0.124

CaHCO3+ 2.697e-005 2.511e-005 -4.569 -4.600 -0.031

CO2 2.601e-005 2.604e-005 -4.585 -4.584 0.000

MgHCO3+ 1.187e-005 1.103e-005 -4.926 -4.958 -0.032

MgCO3 9.957e-006 9.967e-006 -5.002 -5.001 0.000

NaHCO3 1.302e-008 1.303e-008 -7.885 -7.885 0.000

NaCO3- 6.263e-009 5.819e-009 -8.203 -8.235 -0.032

Ca 1.055e-003

Ca+2 9.806e-004 7.359e-004 -3.009 -3.133 -0.125

CaCO3 3.617e-005 3.621e-005 -4.442 -4.441 0.000

CaHCO3+ 2.697e-005 2.511e-005 -4.569 -4.600 -0.031

CaSO4 1.117e-005 1.118e-005 -4.952 -4.952 0.000

CaOH+ 2.684e-008 2.493e-008 -7.571 -7.603 -0.032

CaHSO4+ 3.685e-013 3.424e-013 -12.434 -12.466 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.317e-005 -4.242 -4.274 -0.032

H(0) 3.231e-028

H2 1.615e-028 1.617e-028 -27.792 -27.791 0.000

K 3.325e-006

K+ 3.324e-006 3.086e-006 -5.478 -5.511 -0.032

KSO4- 1.849e-009 1.718e-009 -8.733 -8.765 -0.032

KOH 2.182e-012 2.184e-012 -11.661 -11.661 0.000

Mg 5.184e-004

Mg+2 4.890e-004 3.682e-004 -3.311 -3.434 -0.123

MgHCO3+ 1.187e-005 1.103e-005 -4.926 -4.958 -0.032

MgCO3 9.957e-006 9.967e-006 -5.002 -5.001 0.000

MgSO4 7.115e-006 7.123e-006 -5.148 -5.147 0.000

MgOH+ 4.579e-007 4.255e-007 -6.339 -6.371 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.282e-006 -5.001 -5.032 -0.032

NaHCO3 1.302e-008 1.303e-008 -7.885 -7.885 0.000

NaCO3- 6.263e-009 5.819e-009 -8.203 -8.235 -0.032

NaSO4- 3.756e-009 3.489e-009 -8.425 -8.457 -0.032

NaOH 1.251e-011 1.252e-011 -10.903 -10.902 0.000

O(0) 6.158e-004

O2 3.079e-004 3.082e-004 -3.512 -3.511 0.000

S(6) 1.154e-004

SO4-2 9.708e-005 7.270e-005 -4.013 -4.138 -0.126

CaSO4 1.117e-005 1.118e-005 -4.952 -4.952 0.000

MgSO4 7.115e-006 7.123e-006 -5.148 -5.147 0.000

NaSO4- 3.756e-009 3.489e-009 -8.425 -8.457 -0.032

KSO4- 1.849e-009 1.718e-009 -8.733 -8.765 -0.032

HSO4- 4.165e-011 3.870e-011 -10.380 -10.412 -0.032

CaHSO4+ 3.685e-013 3.424e-013 -12.434 -12.466 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.27 -4.39 CaSO4

Aragonite 0.66 -7.71 -8.37 CaCO3

Calcite 0.80 -7.71 -8.51 CaCO3

CO2(g) -3.06 -4.58 -1.52 CO2

Dolomite 1.48 -15.73 -17.20 CaMg(CO3)2

Gypsum -2.69 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.62 -27.79 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.58 -3.51 -2.93 O2

Initial solution 9. 29/8/2012 13:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.907e-003 2.907e-003

Ca 1.062e-003 1.062e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.545e-004 6.545e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.340

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 322

Density (g/cm3) = 0.99589

Activity of water = 1.000

Ionic strength = 4.618e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.841e-003

Total CO2 (mol/kg) = 2.841e-003

Temperature (deg C) = 29.900

Electrical balance (eq) = -2.047e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.34

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551583e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9095 0.7161

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.386e-006 3.143e-006 -5.470 -5.503 -0.032

H+ 4.887e-009 4.571e-009 -8.311 -8.340 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.841e-003

HCO3- 2.690e-003 2.504e-003 -2.570 -2.601 -0.031

CaCO3 3.888e-005 3.892e-005 -4.410 -4.410 0.000

CO3-2 3.755e-005 2.818e-005 -4.425 -4.550 -0.125

CaHCO3+ 2.713e-005 2.526e-005 -4.566 -4.598 -0.031

CO2 2.437e-005 2.439e-005 -4.613 -4.613 0.000

MgHCO3+ 1.188e-005 1.103e-005 -4.925 -4.957 -0.032

MgCO3 1.065e-005 1.066e-005 -4.973 -4.972 0.000

NaHCO3 1.306e-008 1.307e-008 -7.884 -7.884 0.000

NaCO3- 6.686e-009 6.211e-009 -8.175 -8.207 -0.032

Ca 1.062e-003

Ca+2 9.852e-004 7.391e-004 -3.006 -3.131 -0.125

CaCO3 3.888e-005 3.892e-005 -4.410 -4.410 0.000

CaHCO3+ 2.713e-005 2.526e-005 -4.566 -4.598 -0.031

CaSO4 1.120e-005 1.121e-005 -4.951 -4.950 0.000

CaOH+ 2.888e-008 2.683e-008 -7.539 -7.571 -0.032

CaHSO4+ 3.445e-013 3.200e-013 -12.463 -12.495 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.317e-005 -4.242 -4.274 -0.032

H(0) 2.817e-028

H2 1.408e-028 1.410e-028 -27.851 -27.851 0.000

K 3.325e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.845e-009 1.714e-009 -8.734 -8.766 -0.032

KOH 2.338e-012 2.340e-012 -11.631 -11.631 0.000

Mg 5.184e-004

Mg+2 4.883e-004 3.675e-004 -3.311 -3.435 -0.123

MgHCO3+ 1.188e-005 1.103e-005 -4.925 -4.957 -0.032

MgCO3 1.065e-005 1.066e-005 -4.973 -4.972 0.000

MgSO4 7.081e-006 7.089e-006 -5.150 -5.149 0.000

MgOH+ 4.856e-007 4.511e-007 -6.314 -6.346 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.281e-006 -5.001 -5.032 -0.032

NaHCO3 1.306e-008 1.307e-008 -7.884 -7.884 0.000

NaCO3- 6.686e-009 6.211e-009 -8.175 -8.207 -0.032

NaSO4- 3.752e-009 3.485e-009 -8.426 -8.458 -0.032

NaOH 1.340e-011 1.341e-011 -10.873 -10.872 0.000

O(0) 6.545e-004

O2 3.273e-004 3.276e-004 -3.485 -3.485 0.000

S(6) 1.154e-004

SO4-2 9.708e-005 7.267e-005 -4.013 -4.139 -0.126

CaSO4 1.120e-005 1.121e-005 -4.951 -4.950 0.000

MgSO4 7.081e-006 7.089e-006 -5.150 -5.149 0.000

NaSO4- 3.752e-009 3.485e-009 -8.426 -8.458 -0.032

KSO4- 1.845e-009 1.714e-009 -8.734 -8.766 -0.032

HSO4- 3.877e-011 3.602e-011 -10.412 -10.444 -0.032

CaHSO4+ 3.445e-013 3.200e-013 -12.463 -12.495 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.69 -7.68 -8.37 CaCO3

Calcite 0.83 -7.68 -8.51 CaCO3

CO2(g) -3.09 -4.61 -1.52 CO2

Dolomite 1.54 -15.67 -17.20 CaMg(CO3)2

Gypsum -2.69 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.68 -27.85 -3.17 H2

H2O(g) -1.39 -0.00 1.39 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.56 -3.48 -2.93 O2

Initial solution 10. 29/8/2012 14:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.907e-003 2.907e-003

Ca 1.062e-003 1.062e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.351e-004 5.351e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.370

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 322

Density (g/cm3) = 0.99585

Activity of water = 1.000

Ionic strength = 4.611e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.833e-003

Total CO2 (mol/kg) = 2.833e-003

Temperature (deg C) = 30.000

Electrical balance (eq) = -2.047e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.34

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551569e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8496 0.7127

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.655e-006 3.392e-006 -5.437 -5.470 -0.032

H+ 4.561e-009 4.266e-009 -8.341 -8.370 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.833e-003

HCO3- 2.678e-003 2.493e-003 -2.572 -2.603 -0.031

CaCO3 4.154e-005 4.159e-005 -4.381 -4.381 0.000

CO3-2 4.012e-005 3.012e-005 -4.397 -4.521 -0.125

CaHCO3+ 2.698e-005 2.511e-005 -4.569 -4.600 -0.031

CO2 2.262e-005 2.264e-005 -4.646 -4.645 0.000

MgHCO3+ 1.181e-005 1.097e-005 -4.928 -4.960 -0.032

MgCO3 1.138e-005 1.139e-005 -4.944 -4.943 0.000

NaHCO3 1.300e-008 1.301e-008 -7.886 -7.886 0.000

NaCO3- 7.180e-009 6.670e-009 -8.144 -8.176 -0.032

Ca 1.062e-003

Ca+2 9.827e-004 7.373e-004 -3.008 -3.132 -0.125

CaCO3 4.154e-005 4.159e-005 -4.381 -4.381 0.000

CaHCO3+ 2.698e-005 2.511e-005 -4.569 -4.600 -0.031

CaSO4 1.118e-005 1.120e-005 -4.951 -4.951 0.000

CaOH+ 3.087e-008 2.868e-008 -7.510 -7.542 -0.032

CaHSO4+ 3.215e-013 2.987e-013 -12.493 -12.525 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.317e-005 -4.242 -4.274 -0.032

H(0) 2.451e-028

H2 1.225e-028 1.227e-028 -27.912 -27.911 0.000

K 3.325e-006

K+ 3.324e-006 3.086e-006 -5.478 -5.511 -0.032

KSO4- 1.848e-009 1.717e-009 -8.733 -8.765 -0.032

KOH 2.505e-012 2.508e-012 -11.601 -11.601 0.000

Mg 5.184e-004

Mg+2 4.876e-004 3.670e-004 -3.312 -3.435 -0.123

MgHCO3+ 1.181e-005 1.097e-005 -4.928 -4.960 -0.032

MgCO3 1.138e-005 1.139e-005 -4.944 -4.943 0.000

MgSO4 7.091e-006 7.099e-006 -5.149 -5.149 0.000

MgOH+ 5.242e-007 4.870e-007 -6.281 -6.312 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.281e-006 -5.001 -5.032 -0.032

NaHCO3 1.300e-008 1.301e-008 -7.886 -7.886 0.000

NaCO3- 7.180e-009 6.670e-009 -8.144 -8.176 -0.032

NaSO4- 3.754e-009 3.488e-009 -8.425 -8.457 -0.032

NaOH 1.436e-011 1.437e-011 -10.843 -10.842 0.000

O(0) 5.351e-004

O2 2.676e-004 2.679e-004 -3.573 -3.572 0.000

S(6) 1.154e-004

SO4-2 9.709e-005 7.269e-005 -4.013 -4.139 -0.126

CaSO4 1.118e-005 1.120e-005 -4.951 -4.951 0.000

MgSO4 7.091e-006 7.099e-006 -5.149 -5.149 0.000

NaSO4- 3.754e-009 3.488e-009 -8.425 -8.457 -0.032

KSO4- 1.848e-009 1.717e-009 -8.733 -8.765 -0.032

HSO4- 3.627e-011 3.369e-011 -10.440 -10.472 -0.032

CaHSO4+ 3.215e-013 2.987e-013 -12.493 -12.525 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.27 -4.39 CaSO4

Aragonite 0.72 -7.65 -8.37 CaCO3

Calcite 0.86 -7.65 -8.51 CaCO3

CO2(g) -3.12 -4.65 -1.52 CO2

Dolomite 1.59 -15.61 -17.20 CaMg(CO3)2

Gypsum -2.69 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.74 -27.91 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.65 -3.57 -2.93 O2

Initial solution 11. 29/8/2012 14:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.949e-003 2.949e-003

Ca 1.077e-003 1.077e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.814e-004 5.814e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.320

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 327

Density (g/cm3) = 0.99583

Activity of water = 1.000

Ionic strength = 4.667e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.885e-003

Total CO2 (mol/kg) = 2.885e-003

Temperature (deg C) = 30.100

Electrical balance (eq) = -3.183e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.52

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551589e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9006 0.7160

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.282e-006 3.045e-006 -5.484 -5.516 -0.033

H+ 5.119e-009 4.786e-009 -8.291 -8.320 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.885e-003

HCO3- 2.734e-003 2.544e-003 -2.563 -2.595 -0.031

CaCO3 3.852e-005 3.856e-005 -4.414 -4.414 0.000

CO3-2 3.661e-005 2.744e-005 -4.436 -4.562 -0.125

CaHCO3+ 2.800e-005 2.605e-005 -4.553 -4.584 -0.031

CO2 2.587e-005 2.590e-005 -4.587 -4.587 0.000

MgHCO3+ 1.207e-005 1.120e-005 -4.918 -4.951 -0.032

MgCO3 1.038e-005 1.039e-005 -4.984 -4.983 0.000

NaHCO3 1.326e-008 1.327e-008 -7.878 -7.877 0.000

NaCO3- 6.573e-009 6.104e-009 -8.182 -8.214 -0.032

Ca 1.077e-003

Ca+2 9.995e-004 7.487e-004 -3.000 -3.126 -0.125

CaCO3 3.852e-005 3.856e-005 -4.414 -4.414 0.000

CaHCO3+ 2.800e-005 2.605e-005 -4.553 -4.584 -0.031

CaSO4 1.133e-005 1.134e-005 -4.946 -4.945 0.000

CaOH+ 2.795e-008 2.596e-008 -7.554 -7.586 -0.032

CaHSO4+ 3.661e-013 3.400e-013 -12.436 -12.468 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.275 -0.032

H(0) 3.082e-028

H2 1.541e-028 1.543e-028 -27.812 -27.812 0.000

K 3.325e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.846e-009 1.714e-009 -8.734 -8.766 -0.032

KOH 2.232e-012 2.234e-012 -11.651 -11.651 0.000

Mg 5.184e-004

Mg+2 4.884e-004 3.671e-004 -3.311 -3.435 -0.124

MgHCO3+ 1.207e-005 1.120e-005 -4.918 -4.951 -0.032

MgCO3 1.038e-005 1.039e-005 -4.984 -4.983 0.000

MgSO4 7.087e-006 7.095e-006 -5.150 -5.149 0.000

MgOH+ 4.715e-007 4.379e-007 -6.327 -6.359 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.326e-008 1.327e-008 -7.878 -7.877 0.000

NaCO3- 6.573e-009 6.104e-009 -8.182 -8.214 -0.032

NaSO4- 3.745e-009 3.478e-009 -8.427 -8.459 -0.032

NaOH 1.279e-011 1.281e-011 -10.893 -10.893 0.000

O(0) 5.814e-004

O2 2.907e-004 2.910e-004 -3.537 -3.536 0.000

S(6) 1.154e-004

SO4-2 9.694e-005 7.246e-005 -4.013 -4.140 -0.126

CaSO4 1.133e-005 1.134e-005 -4.946 -4.945 0.000

MgSO4 7.087e-006 7.095e-006 -5.150 -5.149 0.000

NaSO4- 3.745e-009 3.478e-009 -8.427 -8.459 -0.032

KSO4- 1.846e-009 1.714e-009 -8.734 -8.766 -0.032

HSO4- 4.068e-011 3.777e-011 -10.391 -10.423 -0.032

CaHSO4+ 3.661e-013 3.400e-013 -12.436 -12.468 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.68 -7.69 -8.37 CaCO3

Calcite 0.82 -7.69 -8.51 CaCO3

CO2(g) -3.06 -4.59 -1.53 CO2

Dolomite 1.52 -15.68 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.64 -27.81 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.61 -3.54 -2.93 O2

Initial solution 12. 29/8/2012 14:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.938e-003 2.938e-003

Ca 1.074e-003 1.074e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.389e-004 5.389e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.360

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 326

Density (g/cm3) = 0.99580

Activity of water = 1.000

Ionic strength = 4.646e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.865e-003

Total CO2 (mol/kg) = 2.865e-003

Temperature (deg C) = 30.200

Electrical balance (eq) = -2.899e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.48

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551579e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8444 0.7129

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.624e-006 3.363e-006 -5.441 -5.473 -0.032

H+ 4.668e-009 4.365e-009 -8.331 -8.360 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.865e-003

HCO3- 2.709e-003 2.521e-003 -2.567 -2.598 -0.031

CaCO3 4.177e-005 4.182e-005 -4.379 -4.379 0.000

CO3-2 3.983e-005 2.987e-005 -4.400 -4.525 -0.125

CaHCO3+ 2.761e-005 2.569e-005 -4.559 -4.590 -0.031

CO2 2.336e-005 2.338e-005 -4.632 -4.631 0.000

MgHCO3+ 1.195e-005 1.110e-005 -4.923 -4.955 -0.032

MgCO3 1.130e-005 1.132e-005 -4.947 -4.946 0.000

NaHCO3 1.314e-008 1.315e-008 -7.881 -7.881 0.000

NaCO3- 7.189e-009 6.677e-009 -8.143 -8.175 -0.032

Ca 1.074e-003

Ca+2 9.929e-004 7.442e-004 -3.003 -3.128 -0.125

CaCO3 4.177e-005 4.182e-005 -4.379 -4.379 0.000

CaHCO3+ 2.761e-005 2.569e-005 -4.559 -4.590 -0.031

CaSO4 1.128e-005 1.130e-005 -4.948 -4.947 0.000

CaOH+ 3.046e-008 2.829e-008 -7.516 -7.548 -0.032

CaHSO4+ 3.329e-013 3.092e-013 -12.478 -12.510 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.274 -0.032

H(0) 2.561e-028

H2 1.281e-028 1.282e-028 -27.893 -27.892 0.000

K 3.325e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.850e-009 1.719e-009 -8.733 -8.765 -0.032

KOH 2.447e-012 2.450e-012 -11.611 -11.611 0.000

Mg 5.184e-004

Mg+2 4.875e-004 3.666e-004 -3.312 -3.436 -0.124

MgHCO3+ 1.195e-005 1.110e-005 -4.923 -4.955 -0.032

MgCO3 1.130e-005 1.132e-005 -4.947 -4.946 0.000

MgSO4 7.102e-006 7.110e-006 -5.149 -5.148 0.000

MgOH+ 5.208e-007 4.837e-007 -6.283 -6.315 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.278e-006 -5.001 -5.033 -0.032

NaHCO3 1.314e-008 1.315e-008 -7.881 -7.881 0.000

NaCO3- 7.189e-009 6.677e-009 -8.143 -8.175 -0.032

NaSO4- 3.751e-009 3.484e-009 -8.426 -8.458 -0.032

NaOH 1.403e-011 1.404e-011 -10.853 -10.853 0.000

O(0) 5.389e-004

O2 2.694e-004 2.697e-004 -3.570 -3.569 0.000

S(6) 1.154e-004

SO4-2 9.698e-005 7.253e-005 -4.013 -4.140 -0.126

CaSO4 1.128e-005 1.130e-005 -4.948 -4.947 0.000

MgSO4 7.102e-006 7.110e-006 -5.149 -5.148 0.000

NaSO4- 3.751e-009 3.484e-009 -8.426 -8.458 -0.032

KSO4- 1.850e-009 1.719e-009 -8.733 -8.765 -0.032

HSO4- 3.721e-011 3.456e-011 -10.429 -10.461 -0.032

CaHSO4+ 3.329e-013 3.092e-013 -12.478 -12.510 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.72 -7.65 -8.37 CaCO3

Calcite 0.86 -7.65 -8.51 CaCO3

CO2(g) -3.10 -4.63 -1.53 CO2

Dolomite 1.59 -15.61 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.72 -27.89 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.64 -3.57 -2.93 O2

Initial solution 13. 29/8/2012 14:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.077e-004 6.077e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.340

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 332

Density (g/cm3) = 0.99580

Activity of water = 1.000

Ionic strength = 4.731e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.940e-003

Total CO2 (mol/kg) = 2.940e-003

Temperature (deg C) = 30.200

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.79

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551608e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8774 0.7149

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.463e-006 3.211e-006 -5.461 -5.493 -0.033

H+ 4.891e-009 4.571e-009 -8.311 -8.340 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.940e-003

HCO3- 2.781e-003 2.587e-003 -2.556 -2.587 -0.031

CaCO3 4.185e-005 4.190e-005 -4.378 -4.378 0.000

CO3-2 3.912e-005 2.927e-005 -4.408 -4.534 -0.126

CaHCO3+ 2.898e-005 2.696e-005 -4.538 -4.569 -0.031

CO2 2.510e-005 2.513e-005 -4.600 -4.600 0.000

MgHCO3+ 1.224e-005 1.136e-005 -4.912 -4.945 -0.032

MgCO3 1.105e-005 1.107e-005 -4.956 -4.956 0.000

NaHCO3 1.347e-008 1.349e-008 -7.871 -7.870 0.000

NaCO3- 7.045e-009 6.540e-009 -8.152 -8.184 -0.032

Ca 1.100e-003

Ca+2 1.017e-003 7.608e-004 -2.992 -3.119 -0.126

CaCO3 4.185e-005 4.190e-005 -4.378 -4.378 0.000

CaHCO3+ 2.898e-005 2.696e-005 -4.538 -4.569 -0.031

CaSO4 1.149e-005 1.150e-005 -4.940 -4.939 0.000

CaOH+ 2.976e-008 2.762e-008 -7.526 -7.559 -0.032

CaHSO4+ 3.552e-013 3.297e-013 -12.450 -12.482 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 2.808e-028

H2 1.404e-028 1.406e-028 -27.853 -27.852 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.843e-009 1.711e-009 -8.735 -8.767 -0.032

KOH 2.336e-012 2.338e-012 -11.632 -11.631 0.000

Mg 5.184e-004

Mg+2 4.876e-004 3.658e-004 -3.312 -3.437 -0.125

MgHCO3+ 1.224e-005 1.136e-005 -4.912 -4.945 -0.032

MgCO3 1.105e-005 1.107e-005 -4.956 -4.956 0.000

MgSO4 7.058e-006 7.065e-006 -5.151 -5.151 0.000

MgOH+ 4.966e-007 4.609e-007 -6.304 -6.336 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.272e-006 -5.001 -5.033 -0.032

NaHCO3 1.347e-008 1.349e-008 -7.871 -7.870 0.000

NaCO3- 7.045e-009 6.540e-009 -8.152 -8.184 -0.032

NaSO4- 3.736e-009 3.467e-009 -8.428 -8.460 -0.032

NaOH 1.339e-011 1.340e-011 -10.873 -10.873 0.000

O(0) 6.077e-004

O2 3.038e-004 3.042e-004 -3.517 -3.517 0.000

S(6) 1.154e-004

SO4-2 9.682e-005 7.223e-005 -4.014 -4.141 -0.127

CaSO4 1.149e-005 1.150e-005 -4.940 -4.939 0.000

MgSO4 7.058e-006 7.065e-006 -5.151 -5.151 0.000

NaSO4- 3.736e-009 3.467e-009 -8.428 -8.460 -0.032

KSO4- 1.843e-009 1.711e-009 -8.735 -8.767 -0.032

HSO4- 3.883e-011 3.604e-011 -10.411 -10.443 -0.032

CaHSO4+ 3.552e-013 3.297e-013 -12.450 -12.482 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.87 -7.26 -4.39 CaSO4

Aragonite 0.72 -7.65 -8.37 CaCO3

Calcite 0.86 -7.65 -8.51 CaCO3

CO2(g) -3.07 -4.60 -1.53 CO2

Dolomite 1.59 -15.62 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.68 -27.85 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.59 -3.52 -2.93 O2

Initial solution 14. 29/8/2012 15:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.021e-003 3.021e-003

Ca 1.104e-003 1.104e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.339e-004 5.339e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.340

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 334

Density (g/cm3) = 0.99577

Activity of water = 1.000

Ionic strength = 4.741e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.950e-003

Total CO2 (mol/kg) = 2.950e-003

Temperature (deg C) = 30.300

Electrical balance (eq) = -5.188e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.84

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551604e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8553 0.7138

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.488e-006 3.235e-006 -5.457 -5.490 -0.033

H+ 4.891e-009 4.571e-009 -8.311 -8.340 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.950e-003

HCO3- 2.790e-003 2.595e-003 -2.554 -2.586 -0.032

CaCO3 4.227e-005 4.231e-005 -4.374 -4.374 0.000

CO3-2 3.932e-005 2.941e-005 -4.405 -4.531 -0.126

CaHCO3+ 2.919e-005 2.715e-005 -4.535 -4.566 -0.032

CO2 2.515e-005 2.518e-005 -4.599 -4.599 0.000

MgHCO3+ 1.228e-005 1.140e-005 -4.911 -4.943 -0.032

MgCO3 1.112e-005 1.113e-005 -4.954 -4.954 0.000

NaHCO3 1.351e-008 1.353e-008 -7.869 -7.869 0.000

NaCO3- 7.114e-009 6.603e-009 -8.148 -8.180 -0.032

Ca 1.104e-003

Ca+2 1.021e-003 7.629e-004 -2.991 -3.118 -0.126

CaCO3 4.227e-005 4.231e-005 -4.374 -4.374 0.000

CaHCO3+ 2.919e-005 2.715e-005 -4.535 -4.566 -0.032

CaSO4 1.152e-005 1.153e-005 -4.938 -4.938 0.000

CaOH+ 2.984e-008 2.770e-008 -7.525 -7.558 -0.032

CaHSO4+ 3.567e-013 3.311e-013 -12.448 -12.480 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 2.806e-028

H2 1.403e-028 1.404e-028 -27.853 -27.853 0.000

K 3.326e-006

K+ 3.324e-006 3.082e-006 -5.478 -5.511 -0.033

KSO4- 1.845e-009 1.712e-009 -8.734 -8.767 -0.032

KOH 2.336e-012 2.338e-012 -11.632 -11.631 0.000

Mg 5.184e-004

Mg+2 4.874e-004 3.656e-004 -3.312 -3.437 -0.125

MgHCO3+ 1.228e-005 1.140e-005 -4.911 -4.943 -0.032

MgCO3 1.112e-005 1.113e-005 -4.954 -4.954 0.000

MgSO4 7.066e-006 7.074e-006 -5.151 -5.150 0.000

MgOH+ 5.007e-007 4.647e-007 -6.300 -6.333 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.271e-006 -5.001 -5.033 -0.032

NaHCO3 1.351e-008 1.353e-008 -7.869 -7.869 0.000

NaCO3- 7.114e-009 6.603e-009 -8.148 -8.180 -0.032

NaSO4- 3.735e-009 3.467e-009 -8.428 -8.460 -0.032

NaOH 1.339e-011 1.340e-011 -10.873 -10.873 0.000

O(0) 5.339e-004

O2 2.669e-004 2.672e-004 -3.574 -3.573 0.000

S(6) 1.154e-004

SO4-2 9.678e-005 7.218e-005 -4.014 -4.142 -0.127

CaSO4 1.152e-005 1.153e-005 -4.938 -4.938 0.000

MgSO4 7.066e-006 7.074e-006 -5.151 -5.150 0.000

NaSO4- 3.735e-009 3.467e-009 -8.428 -8.460 -0.032

KSO4- 1.845e-009 1.712e-009 -8.734 -8.767 -0.032

HSO4- 3.889e-011 3.610e-011 -10.410 -10.443 -0.032

CaHSO4+ 3.567e-013 3.311e-013 -12.448 -12.480 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.87 -7.26 -4.39 CaSO4

Aragonite 0.72 -7.65 -8.37 CaCO3

Calcite 0.86 -7.65 -8.51 CaCO3

CO2(g) -3.07 -4.60 -1.53 CO2

Dolomite 1.59 -15.62 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.68 -27.85 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.64 -3.57 -2.93 O2

Initial solution 15. 29/8/2012 15:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.021e-003 3.021e-003

Ca 1.104e-003 1.104e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.570e-004 5.570e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.310

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 334

Density (g/cm3) = 0.99577

Activity of water = 1.000

Ionic strength = 4.748e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.957e-003

Total CO2 (mol/kg) = 2.957e-003

Temperature (deg C) = 30.300

Electrical balance (eq) = -5.188e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.84

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551608e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8899 0.7159

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.256e-006 3.019e-006 -5.487 -5.520 -0.033

H+ 5.241e-009 4.898e-009 -8.281 -8.310 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.957e-003

HCO3- 2.802e-003 2.605e-003 -2.553 -2.584 -0.032

CaCO3 3.969e-005 3.974e-005 -4.401 -4.401 0.000

CO3-2 3.686e-005 2.756e-005 -4.434 -4.560 -0.126

CaHCO3+ 2.937e-005 2.731e-005 -4.532 -4.564 -0.032

CO2 2.706e-005 2.709e-005 -4.568 -4.567 0.000

MgHCO3+ 1.234e-005 1.146e-005 -4.909 -4.941 -0.032

MgCO3 1.043e-005 1.044e-005 -4.982 -4.981 0.000

NaHCO3 1.357e-008 1.358e-008 -7.867 -7.867 0.000

NaCO3- 6.666e-009 6.187e-009 -8.176 -8.209 -0.032

Ca 1.104e-003

Ca+2 1.023e-003 7.645e-004 -2.990 -3.117 -0.126

CaCO3 3.969e-005 3.974e-005 -4.401 -4.401 0.000

CaHCO3+ 2.937e-005 2.731e-005 -4.532 -4.564 -0.032

CaSO4 1.154e-005 1.155e-005 -4.938 -4.937 0.000

CaOH+ 2.791e-008 2.590e-008 -7.554 -7.587 -0.032

CaHSO4+ 3.829e-013 3.554e-013 -12.417 -12.449 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.311e-005 -4.242 -4.275 -0.033

H(0) 3.221e-028

H2 1.611e-028 1.612e-028 -27.793 -27.793 0.000

K 3.326e-006

K+ 3.324e-006 3.082e-006 -5.478 -5.511 -0.033

KSO4- 1.844e-009 1.711e-009 -8.734 -8.767 -0.032

KOH 2.180e-012 2.182e-012 -11.662 -11.661 0.000

Mg 5.184e-004

Mg+2 4.881e-004 3.660e-004 -3.312 -3.437 -0.125

MgHCO3+ 1.234e-005 1.146e-005 -4.909 -4.941 -0.032

MgCO3 1.043e-005 1.044e-005 -4.982 -4.981 0.000

MgSO4 7.071e-006 7.079e-006 -5.151 -5.150 0.000

MgOH+ 4.678e-007 4.342e-007 -6.330 -6.362 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.271e-006 -5.001 -5.033 -0.032

NaHCO3 1.357e-008 1.358e-008 -7.867 -7.867 0.000

NaCO3- 6.666e-009 6.187e-009 -8.176 -8.209 -0.032

NaSO4- 3.733e-009 3.465e-009 -8.428 -8.460 -0.032

NaOH 1.249e-011 1.251e-011 -10.903 -10.903 0.000

O(0) 5.570e-004

O2 2.785e-004 2.788e-004 -3.555 -3.555 0.000

S(6) 1.154e-004

SO4-2 9.675e-005 7.215e-005 -4.014 -4.142 -0.127

CaSO4 1.154e-005 1.155e-005 -4.938 -4.937 0.000

MgSO4 7.071e-006 7.079e-006 -5.151 -5.150 0.000

NaSO4- 3.733e-009 3.465e-009 -8.428 -8.460 -0.032

KSO4- 1.844e-009 1.711e-009 -8.734 -8.767 -0.032

HSO4- 4.166e-011 3.866e-011 -10.380 -10.413 -0.032

CaHSO4+ 3.829e-013 3.554e-013 -12.417 -12.449 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.87 -7.26 -4.39 CaSO4

Aragonite 0.70 -7.68 -8.37 CaCO3

Calcite 0.84 -7.68 -8.51 CaCO3

CO2(g) -3.04 -4.57 -1.53 CO2

Dolomite 1.54 -15.67 -17.21 CaMg(CO3)2

Gypsum -2.67 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.62 -27.79 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.63 -3.55 -2.93 O2

Initial solution 16. 29/8/2012 15:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.439e-004 5.439e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.360

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 332

Density (g/cm3) = 0.99580

Activity of water = 1.000

Ionic strength = 4.726e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.934e-003

Total CO2 (mol/kg) = 2.934e-003

Temperature (deg C) = 30.200

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.79

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551601e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8454 0.7129

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.626e-006 3.363e-006 -5.441 -5.473 -0.033

H+ 4.670e-009 4.365e-009 -8.331 -8.360 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.934e-003

HCO3- 2.773e-003 2.579e-003 -2.557 -2.588 -0.031

CaCO3 4.364e-005 4.368e-005 -4.360 -4.360 0.000

CO3-2 4.084e-005 3.056e-005 -4.389 -4.515 -0.126

CaHCO3+ 2.886e-005 2.684e-005 -4.540 -4.571 -0.031

CO2 2.390e-005 2.393e-005 -4.622 -4.621 0.000

MgHCO3+ 1.219e-005 1.132e-005 -4.914 -4.946 -0.032

MgCO3 1.153e-005 1.154e-005 -4.938 -4.938 0.000

NaHCO3 1.344e-008 1.345e-008 -7.872 -7.871 0.000

NaCO3- 7.356e-009 6.828e-009 -8.133 -8.166 -0.032

Ca 1.100e-003

Ca+2 1.016e-003 7.597e-004 -2.993 -3.119 -0.126

CaCO3 4.364e-005 4.368e-005 -4.360 -4.360 0.000

CaHCO3+ 2.886e-005 2.684e-005 -4.540 -4.571 -0.031

CaSO4 1.148e-005 1.149e-005 -4.940 -4.940 0.000

CaOH+ 3.111e-008 2.888e-008 -7.507 -7.539 -0.032

CaHSO4+ 3.388e-013 3.145e-013 -12.470 -12.502 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 2.561e-028

H2 1.281e-028 1.282e-028 -27.893 -27.892 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.843e-009 1.711e-009 -8.734 -8.767 -0.032

KOH 2.446e-012 2.449e-012 -11.612 -11.611 0.000

Mg 5.184e-004

Mg+2 4.871e-004 3.655e-004 -3.312 -3.437 -0.125

MgHCO3+ 1.219e-005 1.132e-005 -4.914 -4.946 -0.032

MgCO3 1.153e-005 1.154e-005 -4.938 -4.938 0.000

MgSO4 7.054e-006 7.062e-006 -5.152 -5.151 0.000

MgOH+ 5.195e-007 4.823e-007 -6.284 -6.317 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.272e-006 -5.001 -5.033 -0.032

NaHCO3 1.344e-008 1.345e-008 -7.872 -7.871 0.000

NaCO3- 7.356e-009 6.828e-009 -8.133 -8.166 -0.032

NaSO4- 3.737e-009 3.469e-009 -8.428 -8.460 -0.032

NaOH 1.402e-011 1.403e-011 -10.853 -10.853 0.000

O(0) 5.439e-004

O2 2.719e-004 2.722e-004 -3.566 -3.565 0.000

S(6) 1.154e-004

SO4-2 9.683e-005 7.226e-005 -4.014 -4.141 -0.127

CaSO4 1.148e-005 1.149e-005 -4.940 -4.940 0.000

MgSO4 7.054e-006 7.062e-006 -5.152 -5.151 0.000

NaSO4- 3.737e-009 3.469e-009 -8.428 -8.460 -0.032

KSO4- 1.843e-009 1.711e-009 -8.734 -8.767 -0.032

HSO4- 3.709e-011 3.443e-011 -10.431 -10.463 -0.032

CaHSO4+ 3.388e-013 3.145e-013 -12.470 -12.502 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.87 -7.26 -4.39 CaSO4

Aragonite 0.74 -7.63 -8.37 CaCO3

Calcite 0.88 -7.63 -8.51 CaCO3

CO2(g) -3.09 -4.62 -1.53 CO2

Dolomite 1.62 -15.59 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.72 -27.89 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.64 -3.57 -2.93 O2

Initial solution 17. 29/8/2012 15:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.108e-004 5.108e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.380

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 330

Density (g/cm3) = 0.99583

Activity of water = 1.000

Ionic strength = 4.710e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.919e-003

Total CO2 (mol/kg) = 2.919e-003

Temperature (deg C) = 30.100

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.75

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551593e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8265 0.7116

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.769e-006 3.496e-006 -5.424 -5.456 -0.033

H+ 4.460e-009 4.169e-009 -8.351 -8.380 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.919e-003

HCO3- 2.756e-003 2.564e-003 -2.560 -2.591 -0.031

CaCO3 4.504e-005 4.509e-005 -4.346 -4.346 0.000

CO3-2 4.242e-005 3.175e-005 -4.372 -4.498 -0.126

CaHCO3+ 2.853e-005 2.653e-005 -4.545 -4.576 -0.031

CO2 2.271e-005 2.273e-005 -4.644 -4.643 0.000

MgHCO3+ 1.211e-005 1.124e-005 -4.917 -4.949 -0.032

MgCO3 1.196e-005 1.197e-005 -4.922 -4.922 0.000

NaHCO3 1.336e-008 1.337e-008 -7.874 -7.874 0.000

NaCO3- 7.606e-009 7.061e-009 -8.119 -8.151 -0.032

Ca 1.096e-003

Ca+2 1.011e-003 7.565e-004 -2.995 -3.121 -0.126

CaCO3 4.504e-005 4.509e-005 -4.346 -4.346 0.000

CaHCO3+ 2.853e-005 2.653e-005 -4.545 -4.576 -0.031

CaSO4 1.143e-005 1.144e-005 -4.942 -4.942 0.000

CaOH+ 3.244e-008 3.011e-008 -7.489 -7.521 -0.032

CaHSO4+ 3.217e-013 2.987e-013 -12.492 -12.525 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 2.338e-028

H2 1.169e-028 1.170e-028 -27.932 -27.932 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.842e-009 1.710e-009 -8.735 -8.767 -0.032

KOH 2.562e-012 2.564e-012 -11.592 -11.591 0.000

Mg 5.184e-004

Mg+2 4.867e-004 3.654e-004 -3.313 -3.437 -0.125

MgHCO3+ 1.211e-005 1.124e-005 -4.917 -4.949 -0.032

MgCO3 1.196e-005 1.197e-005 -4.922 -4.922 0.000

MgSO4 7.043e-006 7.050e-006 -5.152 -5.152 0.000

MgOH+ 5.391e-007 5.005e-007 -6.268 -6.301 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.273e-006 -5.001 -5.033 -0.032

NaHCO3 1.336e-008 1.337e-008 -7.874 -7.874 0.000

NaCO3- 7.606e-009 7.061e-009 -8.119 -8.151 -0.032

NaSO4- 3.738e-009 3.471e-009 -8.427 -8.460 -0.032

NaOH 1.468e-011 1.470e-011 -10.833 -10.833 0.000

O(0) 5.108e-004

O2 2.554e-004 2.557e-004 -3.593 -3.592 0.000

S(6) 1.154e-004

SO4-2 9.689e-005 7.234e-005 -4.014 -4.141 -0.127

CaSO4 1.143e-005 1.144e-005 -4.942 -4.942 0.000

MgSO4 7.043e-006 7.050e-006 -5.152 -5.152 0.000

NaSO4- 3.738e-009 3.471e-009 -8.427 -8.460 -0.032

KSO4- 1.842e-009 1.710e-009 -8.735 -8.767 -0.032

HSO4- 3.538e-011 3.284e-011 -10.451 -10.484 -0.032

CaHSO4+ 3.217e-013 2.987e-013 -12.492 -12.525 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.39 CaSO4

Aragonite 0.75 -7.62 -8.37 CaCO3

Calcite 0.89 -7.62 -8.51 CaCO3

CO2(g) -3.12 -4.64 -1.53 CO2

Dolomite 1.65 -15.55 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.76 -27.93 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.67 -3.59 -2.93 O2

Initial solution 18. 29/8/2012 16:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.033e-004 5.033e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.380

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 330

Density (g/cm3) = 0.99583

Activity of water = 1.000

Ionic strength = 4.710e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.919e-003

Total CO2 (mol/kg) = 2.919e-003

Temperature (deg C) = 30.100

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.75

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551592e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8249 0.7115

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.769e-006 3.496e-006 -5.424 -5.456 -0.033

H+ 4.460e-009 4.169e-009 -8.351 -8.380 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.919e-003

HCO3- 2.756e-003 2.564e-003 -2.560 -2.591 -0.031

CaCO3 4.504e-005 4.509e-005 -4.346 -4.346 0.000

CO3-2 4.242e-005 3.175e-005 -4.372 -4.498 -0.126

CaHCO3+ 2.853e-005 2.653e-005 -4.545 -4.576 -0.031

CO2 2.271e-005 2.273e-005 -4.644 -4.643 0.000

MgHCO3+ 1.211e-005 1.124e-005 -4.917 -4.949 -0.032

MgCO3 1.196e-005 1.197e-005 -4.922 -4.922 0.000

NaHCO3 1.336e-008 1.337e-008 -7.874 -7.874 0.000

NaCO3- 7.606e-009 7.061e-009 -8.119 -8.151 -0.032

Ca 1.096e-003

Ca+2 1.011e-003 7.565e-004 -2.995 -3.121 -0.126

CaCO3 4.504e-005 4.509e-005 -4.346 -4.346 0.000

CaHCO3+ 2.853e-005 2.653e-005 -4.545 -4.576 -0.031

CaSO4 1.143e-005 1.144e-005 -4.942 -4.942 0.000

CaOH+ 3.244e-008 3.011e-008 -7.489 -7.521 -0.032

CaHSO4+ 3.217e-013 2.987e-013 -12.492 -12.525 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 2.338e-028

H2 1.169e-028 1.170e-028 -27.932 -27.932 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.842e-009 1.710e-009 -8.735 -8.767 -0.032

KOH 2.562e-012 2.564e-012 -11.592 -11.591 0.000

Mg 5.184e-004

Mg+2 4.867e-004 3.654e-004 -3.313 -3.437 -0.125

MgHCO3+ 1.211e-005 1.124e-005 -4.917 -4.949 -0.032

MgCO3 1.196e-005 1.197e-005 -4.922 -4.922 0.000

MgSO4 7.043e-006 7.050e-006 -5.152 -5.152 0.000

MgOH+ 5.391e-007 5.005e-007 -6.268 -6.301 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.273e-006 -5.001 -5.033 -0.032

NaHCO3 1.336e-008 1.337e-008 -7.874 -7.874 0.000

NaCO3- 7.606e-009 7.061e-009 -8.119 -8.151 -0.032

NaSO4- 3.738e-009 3.471e-009 -8.427 -8.460 -0.032

NaOH 1.468e-011 1.470e-011 -10.833 -10.833 0.000

O(0) 5.033e-004

O2 2.516e-004 2.519e-004 -3.599 -3.599 0.000

S(6) 1.154e-004

SO4-2 9.689e-005 7.234e-005 -4.014 -4.141 -0.127

CaSO4 1.143e-005 1.144e-005 -4.942 -4.942 0.000

MgSO4 7.043e-006 7.050e-006 -5.152 -5.152 0.000

NaSO4- 3.738e-009 3.471e-009 -8.427 -8.460 -0.032

KSO4- 1.842e-009 1.710e-009 -8.735 -8.767 -0.032

HSO4- 3.538e-011 3.284e-011 -10.451 -10.484 -0.032

CaHSO4+ 3.217e-013 2.987e-013 -12.492 -12.525 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.39 CaSO4

Aragonite 0.75 -7.62 -8.37 CaCO3

Calcite 0.89 -7.62 -8.51 CaCO3

CO2(g) -3.12 -4.64 -1.53 CO2

Dolomite 1.65 -15.55 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.76 -27.93 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.67 -3.60 -2.93 O2

Initial solution 19. 29/8/2012 16:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.895e-004 4.895e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.390

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 330

Density (g/cm3) = 0.99583

Activity of water = 1.000

Ionic strength = 4.708e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.917e-003

Total CO2 (mol/kg) = 2.917e-003

Temperature (deg C) = 30.100

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.75

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551590e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8119 0.7107

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.857e-006 3.578e-006 -5.414 -5.446 -0.033

H+ 4.358e-009 4.074e-009 -8.361 -8.390 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.917e-003

HCO3- 2.752e-003 2.560e-003 -2.560 -2.592 -0.031

CaCO3 4.599e-005 4.604e-005 -4.337 -4.337 0.000

CO3-2 4.334e-005 3.244e-005 -4.363 -4.489 -0.126

CaHCO3+ 2.846e-005 2.647e-005 -4.546 -4.577 -0.031

CO2 2.216e-005 2.218e-005 -4.654 -4.654 0.000

MgCO3 1.222e-005 1.223e-005 -4.913 -4.913 0.000

MgHCO3+ 1.209e-005 1.122e-005 -4.918 -4.950 -0.032

NaHCO3 1.334e-008 1.335e-008 -7.875 -7.874 0.000

NaCO3- 7.771e-009 7.215e-009 -8.110 -8.142 -0.032

Ca 1.096e-003

Ca+2 1.010e-003 7.559e-004 -2.996 -3.122 -0.126

CaCO3 4.599e-005 4.604e-005 -4.337 -4.337 0.000

CaHCO3+ 2.846e-005 2.647e-005 -4.546 -4.577 -0.031

CaSO4 1.142e-005 1.143e-005 -4.942 -4.942 0.000

CaOH+ 3.317e-008 3.079e-008 -7.479 -7.512 -0.032

CaHSO4+ 3.142e-013 2.917e-013 -12.503 -12.535 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 2.233e-028

H2 1.116e-028 1.118e-028 -27.952 -27.952 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.843e-009 1.711e-009 -8.735 -8.767 -0.032

KOH 2.621e-012 2.624e-012 -11.581 -11.581 0.000

Mg 5.184e-004

Mg+2 4.865e-004 3.652e-004 -3.313 -3.437 -0.125

MgCO3 1.222e-005 1.223e-005 -4.913 -4.913 0.000

MgHCO3+ 1.209e-005 1.122e-005 -4.918 -4.950 -0.032

MgSO4 7.041e-006 7.048e-006 -5.152 -5.152 0.000

MgOH+ 5.514e-007 5.119e-007 -6.259 -6.291 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.273e-006 -5.001 -5.033 -0.032

NaHCO3 1.334e-008 1.335e-008 -7.875 -7.874 0.000

NaCO3- 7.771e-009 7.215e-009 -8.110 -8.142 -0.032

NaSO4- 3.739e-009 3.471e-009 -8.427 -8.460 -0.032

NaOH 1.502e-011 1.504e-011 -10.823 -10.823 0.000

O(0) 4.895e-004

O2 2.448e-004 2.450e-004 -3.611 -3.611 0.000

S(6) 1.154e-004

SO4-2 9.690e-005 7.235e-005 -4.014 -4.141 -0.127

CaSO4 1.142e-005 1.143e-005 -4.942 -4.942 0.000

MgSO4 7.041e-006 7.048e-006 -5.152 -5.152 0.000

NaSO4- 3.739e-009 3.471e-009 -8.427 -8.460 -0.032

KSO4- 1.843e-009 1.711e-009 -8.735 -8.767 -0.032

HSO4- 3.458e-011 3.210e-011 -10.461 -10.493 -0.032

CaHSO4+ 3.142e-013 2.917e-013 -12.503 -12.535 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.39 CaSO4

Aragonite 0.76 -7.61 -8.37 CaCO3

Calcite 0.90 -7.61 -8.51 CaCO3

CO2(g) -3.13 -4.65 -1.53 CO2

Dolomite 1.67 -15.54 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.78 -27.95 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.68 -3.61 -2.93 O2

Initial solution 20. 29/8/2012 16:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.990e-003 2.990e-003

Ca 1.092e-003 1.092e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.239e-004 5.239e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.390

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 328

Density (g/cm3) = 0.99586

Activity of water = 1.000

Ionic strength = 4.697e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.907e-003

Total CO2 (mol/kg) = 2.907e-003

Temperature (deg C) = 30.000

Electrical balance (eq) = -4.336e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.71

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551591e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8273 0.7114

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.829e-006 3.552e-006 -5.417 -5.450 -0.033

H+ 4.358e-009 4.074e-009 -8.361 -8.390 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.907e-003

HCO3- 2.744e-003 2.553e-003 -2.562 -2.593 -0.031

CaCO3 4.554e-005 4.559e-005 -4.342 -4.341 0.000

CO3-2 4.312e-005 3.229e-005 -4.365 -4.491 -0.126

CaHCO3+ 2.826e-005 2.629e-005 -4.549 -4.580 -0.031

CO2 2.211e-005 2.214e-005 -4.655 -4.655 0.000

MgCO3 1.215e-005 1.216e-005 -4.916 -4.915 0.000

MgHCO3+ 1.205e-005 1.119e-005 -4.919 -4.951 -0.032

NaHCO3 1.330e-008 1.331e-008 -7.876 -7.876 0.000

NaCO3- 7.697e-009 7.146e-009 -8.114 -8.146 -0.032

Ca 1.092e-003

Ca+2 1.007e-003 7.539e-004 -2.997 -3.123 -0.126

CaCO3 4.554e-005 4.559e-005 -4.342 -4.341 0.000

CaHCO3+ 2.826e-005 2.629e-005 -4.549 -4.580 -0.031

CaSO4 1.139e-005 1.140e-005 -4.943 -4.943 0.000

CaOH+ 3.307e-008 3.071e-008 -7.481 -7.513 -0.032

CaHSO4+ 3.129e-013 2.905e-013 -12.505 -12.537 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 2.235e-028

H2 1.118e-028 1.119e-028 -27.952 -27.951 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.841e-009 1.709e-009 -8.735 -8.767 -0.032

KOH 2.621e-012 2.624e-012 -11.581 -11.581 0.000

Mg 5.184e-004

Mg+2 4.866e-004 3.655e-004 -3.313 -3.437 -0.124

MgCO3 1.215e-005 1.216e-005 -4.916 -4.915 0.000

MgHCO3+ 1.205e-005 1.119e-005 -4.919 -4.951 -0.032

MgSO4 7.033e-006 7.040e-006 -5.153 -5.152 0.000

MgOH+ 5.469e-007 5.077e-007 -6.262 -6.294 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.274e-006 -5.001 -5.033 -0.032

NaHCO3 1.330e-008 1.331e-008 -7.876 -7.876 0.000

NaCO3- 7.697e-009 7.146e-009 -8.114 -8.146 -0.032

NaSO4- 3.739e-009 3.472e-009 -8.427 -8.459 -0.032

NaOH 1.502e-011 1.504e-011 -10.823 -10.823 0.000

O(0) 5.239e-004

O2 2.619e-004 2.622e-004 -3.582 -3.581 0.000

S(6) 1.154e-004

SO4-2 9.694e-005 7.240e-005 -4.013 -4.140 -0.127

CaSO4 1.139e-005 1.140e-005 -4.943 -4.943 0.000

MgSO4 7.033e-006 7.040e-006 -5.153 -5.152 0.000

NaSO4- 3.739e-009 3.472e-009 -8.427 -8.459 -0.032

KSO4- 1.841e-009 1.709e-009 -8.735 -8.767 -0.032

HSO4- 3.452e-011 3.205e-011 -10.462 -10.494 -0.032

CaHSO4+ 3.129e-013 2.905e-013 -12.505 -12.537 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.39 CaSO4

Aragonite 0.76 -7.61 -8.37 CaCO3

Calcite 0.90 -7.61 -8.51 CaCO3

CO2(g) -3.13 -4.65 -1.52 CO2

Dolomite 1.66 -15.54 -17.20 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.78 -27.95 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.65 -3.58 -2.93 O2

Initial solution 21. 29/8/2012 16:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.969e-003 2.969e-003

Ca 1.085e-003 1.085e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.083e-004 5.083e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.400

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 327

Density (g/cm3) = 0.99586

Activity of water = 1.000

Ionic strength = 4.672e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.884e-003

Total CO2 (mol/kg) = 2.884e-003

Temperature (deg C) = 30.000

Electrical balance (eq) = -3.751e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.62

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551582e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8140 0.7106

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.918e-006 3.635e-006 -5.407 -5.440 -0.033

H+ 4.258e-009 3.981e-009 -8.371 -8.400 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.884e-003

HCO3- 2.721e-003 2.532e-003 -2.565 -2.597 -0.031

CaCO3 4.592e-005 4.596e-005 -4.338 -4.338 0.000

CO3-2 4.373e-005 3.278e-005 -4.359 -4.484 -0.125

CaHCO3+ 2.784e-005 2.590e-005 -4.555 -4.587 -0.031

CO2 2.144e-005 2.146e-005 -4.669 -4.668 0.000

MgCO3 1.233e-005 1.235e-005 -4.909 -4.908 0.000

MgHCO3+ 1.196e-005 1.110e-005 -4.922 -4.955 -0.032

NaHCO3 1.319e-008 1.321e-008 -7.880 -7.879 0.000

NaCO3- 7.812e-009 7.255e-009 -8.107 -8.139 -0.032

Ca 1.085e-003

Ca+2 9.997e-004 7.488e-004 -3.000 -3.126 -0.125

CaCO3 4.592e-005 4.596e-005 -4.338 -4.338 0.000

CaHCO3+ 2.784e-005 2.590e-005 -4.555 -4.587 -0.031

CaSO4 1.133e-005 1.134e-005 -4.946 -4.945 0.000

CaOH+ 3.361e-008 3.121e-008 -7.473 -7.506 -0.032

CaHSO4+ 3.040e-013 2.823e-013 -12.517 -12.549 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.275 -0.032

H(0) 2.135e-028

H2 1.067e-028 1.068e-028 -27.972 -27.971 0.000

K 3.325e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.843e-009 1.712e-009 -8.734 -8.767 -0.032

KOH 2.683e-012 2.686e-012 -11.571 -11.571 0.000

Mg 5.184e-004

Mg+2 4.865e-004 3.656e-004 -3.313 -3.437 -0.124

MgCO3 1.233e-005 1.235e-005 -4.909 -4.908 0.000

MgHCO3+ 1.196e-005 1.110e-005 -4.922 -4.955 -0.032

MgSO4 7.044e-006 7.052e-006 -5.152 -5.152 0.000

MgOH+ 5.597e-007 5.198e-007 -6.252 -6.284 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.319e-008 1.321e-008 -7.880 -7.879 0.000

NaCO3- 7.812e-009 7.255e-009 -8.107 -8.139 -0.032

NaSO4- 3.744e-009 3.477e-009 -8.427 -8.459 -0.032

NaOH 1.538e-011 1.539e-011 -10.813 -10.813 0.000

O(0) 5.083e-004

O2 2.541e-004 2.544e-004 -3.595 -3.594 0.000

S(6) 1.154e-004

SO4-2 9.699e-005 7.249e-005 -4.013 -4.140 -0.126

CaSO4 1.133e-005 1.134e-005 -4.946 -4.945 0.000

MgSO4 7.044e-006 7.052e-006 -5.152 -5.152 0.000

NaSO4- 3.744e-009 3.477e-009 -8.427 -8.459 -0.032

KSO4- 1.843e-009 1.712e-009 -8.734 -8.767 -0.032

HSO4- 3.377e-011 3.136e-011 -10.471 -10.504 -0.032

CaHSO4+ 3.040e-013 2.823e-013 -12.517 -12.549 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.76 -7.61 -8.37 CaCO3

Calcite 0.90 -7.61 -8.51 CaCO3

CO2(g) -3.14 -4.67 -1.52 CO2

Dolomite 1.67 -15.53 -17.20 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.80 -27.97 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.67 -3.59 -2.93 O2

Initial solution 22. 29/8/2012 17:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.980e-003 2.980e-003

Ca 1.089e-003 1.089e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.776e-004 4.776e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.420

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 326

Density (g/cm3) = 0.99589

Activity of water = 1.000

Ionic strength = 4.679e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.889e-003

Total CO2 (mol/kg) = 2.889e-003

Temperature (deg C) = 29.900

Electrical balance (eq) = -4.035e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.66

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551581e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.7953 0.7092

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 4.073e-006 3.779e-006 -5.390 -5.423 -0.033

H+ 4.066e-009 3.802e-009 -8.391 -8.420 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.889e-003

HCO3- 2.722e-003 2.533e-003 -2.565 -2.596 -0.031

CaCO3 4.797e-005 4.802e-005 -4.319 -4.319 0.000

CO3-2 4.573e-005 3.427e-005 -4.340 -4.465 -0.125

CaHCO3+ 2.786e-005 2.592e-005 -4.555 -4.586 -0.031

CO2 2.050e-005 2.052e-005 -4.688 -4.688 0.000

MgCO3 1.286e-005 1.288e-005 -4.891 -4.890 0.000

MgHCO3+ 1.194e-005 1.109e-005 -4.923 -4.955 -0.032

NaHCO3 1.320e-008 1.321e-008 -7.880 -7.879 0.000

NaCO3- 8.129e-009 7.548e-009 -8.090 -8.122 -0.032

Ca 1.089e-003

Ca+2 1.001e-003 7.500e-004 -2.999 -3.125 -0.126

CaCO3 4.797e-005 4.802e-005 -4.319 -4.319 0.000

CaHCO3+ 2.786e-005 2.592e-005 -4.555 -4.586 -0.031

CaSO4 1.134e-005 1.135e-005 -4.946 -4.945 0.000

CaOH+ 3.525e-008 3.274e-008 -7.453 -7.485 -0.032

CaHSO4+ 2.902e-013 2.694e-013 -12.537 -12.570 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 1.949e-028

H2 9.743e-029 9.753e-029 -28.011 -28.011 0.000

K 3.325e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.840e-009 1.709e-009 -8.735 -8.767 -0.032

KOH 2.809e-012 2.812e-012 -11.551 -11.551 0.000

Mg 5.184e-004

Mg+2 4.860e-004 3.652e-004 -3.313 -3.437 -0.124

MgCO3 1.286e-005 1.288e-005 -4.891 -4.890 0.000

MgHCO3+ 1.194e-005 1.109e-005 -4.923 -4.955 -0.032

MgSO4 7.019e-006 7.026e-006 -5.154 -5.153 0.000

MgOH+ 5.804e-007 5.389e-007 -6.236 -6.268 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.320e-008 1.321e-008 -7.880 -7.879 0.000

NaCO3- 8.129e-009 7.548e-009 -8.090 -8.122 -0.032

NaSO4- 3.742e-009 3.475e-009 -8.427 -8.459 -0.032

NaOH 1.610e-011 1.612e-011 -10.793 -10.793 0.000

O(0) 4.776e-004

O2 2.388e-004 2.391e-004 -3.622 -3.621 0.000

S(6) 1.154e-004

SO4-2 9.701e-005 7.249e-005 -4.013 -4.140 -0.127

CaSO4 1.134e-005 1.135e-005 -4.946 -4.945 0.000

MgSO4 7.019e-006 7.026e-006 -5.154 -5.153 0.000

NaSO4- 3.742e-009 3.475e-009 -8.427 -8.459 -0.032

KSO4- 1.840e-009 1.709e-009 -8.735 -8.767 -0.032

HSO4- 3.218e-011 2.988e-011 -10.492 -10.525 -0.032

CaHSO4+ 2.902e-013 2.694e-013 -12.537 -12.570 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.39 CaSO4

Aragonite 0.78 -7.59 -8.37 CaCO3

Calcite 0.92 -7.59 -8.51 CaCO3

CO2(g) -3.16 -4.69 -1.52 CO2

Dolomite 1.71 -15.49 -17.20 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.84 -28.01 -3.17 H2

H2O(g) -1.39 -0.00 1.39 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.70 -3.62 -2.93 O2

Initial solution 23. 29/8/2012 17:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.014e-004 5.014e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.420

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 325

Density (g/cm3) = 0.99589

Activity of water = 1.000

Ionic strength = 4.656e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.869e-003

Total CO2 (mol/kg) = 2.869e-003

Temperature (deg C) = 29.900

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551577e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8005 0.7095

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 4.072e-006 3.779e-006 -5.390 -5.423 -0.032

H+ 4.066e-009 3.802e-009 -8.391 -8.420 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.869e-003

HCO3- 2.704e-003 2.516e-003 -2.568 -2.599 -0.031

CaCO3 4.738e-005 4.743e-005 -4.324 -4.324 0.000

CO3-2 4.541e-005 3.405e-005 -4.343 -4.468 -0.125

CaHCO3+ 2.751e-005 2.560e-005 -4.560 -4.592 -0.031

CO2 2.036e-005 2.039e-005 -4.691 -4.691 0.000

MgCO3 1.279e-005 1.280e-005 -4.893 -4.893 0.000

MgHCO3+ 1.187e-005 1.102e-005 -4.926 -4.958 -0.032

NaHCO3 1.311e-008 1.313e-008 -7.882 -7.882 0.000

NaCO3- 8.076e-009 7.501e-009 -8.093 -8.125 -0.032

Ca 1.081e-003

Ca+2 9.949e-004 7.456e-004 -3.002 -3.128 -0.125

CaCO3 4.738e-005 4.743e-005 -4.324 -4.324 0.000

CaHCO3+ 2.751e-005 2.560e-005 -4.560 -4.592 -0.031

CaSO4 1.128e-005 1.129e-005 -4.948 -4.947 0.000

CaOH+ 3.504e-008 3.254e-008 -7.455 -7.488 -0.032

CaHSO4+ 2.887e-013 2.681e-013 -12.540 -12.572 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.274 -0.032

H(0) 1.949e-028

H2 9.743e-029 9.753e-029 -28.011 -28.011 0.000

K 3.325e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.842e-009 1.711e-009 -8.735 -8.767 -0.032

KOH 2.810e-012 2.813e-012 -11.551 -11.551 0.000

Mg 5.184e-004

Mg+2 4.861e-004 3.655e-004 -3.313 -3.437 -0.124

MgCO3 1.279e-005 1.280e-005 -4.893 -4.893 0.000

MgHCO3+ 1.187e-005 1.102e-005 -4.926 -4.958 -0.032

MgSO4 7.032e-006 7.040e-006 -5.153 -5.152 0.000

MgOH+ 5.808e-007 5.394e-007 -6.236 -6.268 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.311e-008 1.313e-008 -7.882 -7.882 0.000

NaCO3- 8.076e-009 7.501e-009 -8.093 -8.125 -0.032

NaSO4- 3.746e-009 3.479e-009 -8.426 -8.459 -0.032

NaOH 1.610e-011 1.612e-011 -10.793 -10.793 0.000

O(0) 5.014e-004

O2 2.507e-004 2.510e-004 -3.601 -3.600 0.000

S(6) 1.154e-004

SO4-2 9.705e-005 7.257e-005 -4.013 -4.139 -0.126

CaSO4 1.128e-005 1.129e-005 -4.948 -4.947 0.000

MgSO4 7.032e-006 7.040e-006 -5.153 -5.152 0.000

NaSO4- 3.746e-009 3.479e-009 -8.426 -8.459 -0.032

KSO4- 1.842e-009 1.711e-009 -8.735 -8.767 -0.032

HSO4- 3.221e-011 2.991e-011 -10.492 -10.524 -0.032

CaHSO4+ 2.887e-013 2.681e-013 -12.540 -12.572 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.77 -7.60 -8.37 CaCO3

Calcite 0.91 -7.60 -8.51 CaCO3

CO2(g) -3.17 -4.69 -1.52 CO2

Dolomite 1.70 -15.50 -17.20 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.84 -28.01 -3.17 H2

H2O(g) -1.39 -0.00 1.39 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.67 -3.60 -2.93 O2

Initial solution 24. 29/8/2012 17:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.969e-003 2.969e-003

Ca 1.085e-003 1.085e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.726e-004 4.726e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.420

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 326

Density (g/cm3) = 0.99589

Activity of water = 1.000

Ionic strength = 4.668e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.879e-003

Total CO2 (mol/kg) = 2.879e-003

Temperature (deg C) = 29.900

Electrical balance (eq) = -3.751e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.62

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551577e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.7941 0.7092

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 4.073e-006 3.779e-006 -5.390 -5.423 -0.033

H+ 4.066e-009 3.802e-009 -8.391 -8.420 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.879e-003

HCO3- 2.713e-003 2.524e-003 -2.567 -2.598 -0.031

CaCO3 4.767e-005 4.773e-005 -4.322 -4.321 0.000

CO3-2 4.557e-005 3.416e-005 -4.341 -4.467 -0.125

CaHCO3+ 2.768e-005 2.576e-005 -4.558 -4.589 -0.031

CO2 2.043e-005 2.045e-005 -4.690 -4.689 0.000

MgCO3 1.283e-005 1.284e-005 -4.892 -4.891 0.000

MgHCO3+ 1.190e-005 1.106e-005 -4.924 -4.956 -0.032

NaHCO3 1.315e-008 1.317e-008 -7.881 -7.880 0.000

NaCO3- 8.102e-009 7.524e-009 -8.091 -8.124 -0.032

Ca 1.085e-003

Ca+2 9.982e-004 7.478e-004 -3.001 -3.126 -0.125

CaCO3 4.767e-005 4.773e-005 -4.322 -4.321 0.000

CaHCO3+ 2.768e-005 2.576e-005 -4.558 -4.589 -0.031

CaSO4 1.131e-005 1.132e-005 -4.947 -4.946 0.000

CaOH+ 3.515e-008 3.264e-008 -7.454 -7.486 -0.032

CaHSO4+ 2.894e-013 2.688e-013 -12.538 -12.571 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.275 -0.032

H(0) 1.949e-028

H2 9.743e-029 9.753e-029 -28.011 -28.011 0.000

K 3.325e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.841e-009 1.710e-009 -8.735 -8.767 -0.032

KOH 2.810e-012 2.813e-012 -11.551 -11.551 0.000

Mg 5.184e-004

Mg+2 4.861e-004 3.653e-004 -3.313 -3.437 -0.124

MgCO3 1.283e-005 1.284e-005 -4.892 -4.891 0.000

MgHCO3+ 1.190e-005 1.106e-005 -4.924 -4.956 -0.032

MgSO4 7.026e-006 7.033e-006 -5.153 -5.153 0.000

MgOH+ 5.806e-007 5.392e-007 -6.236 -6.268 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.315e-008 1.317e-008 -7.881 -7.880 0.000

NaCO3- 8.102e-009 7.524e-009 -8.091 -8.124 -0.032

NaSO4- 3.744e-009 3.477e-009 -8.427 -8.459 -0.032

NaOH 1.610e-011 1.612e-011 -10.793 -10.793 0.000

O(0) 4.726e-004

O2 2.363e-004 2.366e-004 -3.627 -3.626 0.000

S(6) 1.154e-004

SO4-2 9.703e-005 7.253e-005 -4.013 -4.139 -0.126

CaSO4 1.131e-005 1.132e-005 -4.947 -4.946 0.000

MgSO4 7.026e-006 7.033e-006 -5.153 -5.153 0.000

NaSO4- 3.744e-009 3.477e-009 -8.427 -8.459 -0.032

KSO4- 1.841e-009 1.710e-009 -8.735 -8.767 -0.032

HSO4- 3.219e-011 2.990e-011 -10.492 -10.524 -0.032

CaHSO4+ 2.894e-013 2.688e-013 -12.538 -12.571 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.78 -7.59 -8.37 CaCO3

Calcite 0.92 -7.59 -8.51 CaCO3

CO2(g) -3.17 -4.69 -1.52 CO2

Dolomite 1.71 -15.50 -17.20 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.84 -28.01 -3.17 H2

H2O(g) -1.39 -0.00 1.39 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.70 -3.63 -2.93 O2

Initial solution 25. 29/8/2012 17:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.969e-003 2.969e-003

Ca 1.085e-003 1.085e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.782e-004 4.782e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.420

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 325

Density (g/cm3) = 0.99592

Activity of water = 1.000

Ionic strength = 4.668e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.879e-003

Total CO2 (mol/kg) = 2.879e-003

Temperature (deg C) = 29.800

Electrical balance (eq) = -3.751e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.62

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551578e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8034 0.7095

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 4.044e-006 3.752e-006 -5.393 -5.426 -0.033

H+ 4.066e-009 3.802e-009 -8.391 -8.420 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.879e-003

HCO3- 2.714e-003 2.525e-003 -2.566 -2.598 -0.031

CaCO3 4.750e-005 4.755e-005 -4.323 -4.323 0.000

CO3-2 4.550e-005 3.411e-005 -4.342 -4.467 -0.125

CaHCO3+ 2.766e-005 2.574e-005 -4.558 -4.589 -0.031

CO2 2.045e-005 2.048e-005 -4.689 -4.689 0.000

MgCO3 1.279e-005 1.280e-005 -4.893 -4.893 0.000

MgHCO3+ 1.190e-005 1.105e-005 -4.924 -4.956 -0.032

NaHCO3 1.316e-008 1.317e-008 -7.881 -7.880 0.000

NaCO3- 8.050e-009 7.476e-009 -8.094 -8.126 -0.032

Ca 1.085e-003

Ca+2 9.984e-004 7.480e-004 -3.001 -3.126 -0.125

CaCO3 4.750e-005 4.755e-005 -4.323 -4.323 0.000

CaHCO3+ 2.766e-005 2.574e-005 -4.558 -4.589 -0.031

CaSO4 1.130e-005 1.132e-005 -4.947 -4.946 0.000

CaOH+ 3.515e-008 3.265e-008 -7.454 -7.486 -0.032

CaHSO4+ 2.889e-013 2.683e-013 -12.539 -12.571 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.275 -0.032

H(0) 1.950e-028

H2 9.752e-029 9.763e-029 -28.011 -28.010 0.000

K 3.325e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.838e-009 1.707e-009 -8.736 -8.768 -0.032

KOH 2.810e-012 2.813e-012 -11.551 -11.551 0.000

Mg 5.184e-004

Mg+2 4.861e-004 3.654e-004 -3.313 -3.437 -0.124

MgCO3 1.279e-005 1.280e-005 -4.893 -4.893 0.000

MgHCO3+ 1.190e-005 1.105e-005 -4.924 -4.956 -0.032

MgSO4 7.011e-006 7.018e-006 -5.154 -5.154 0.000

MgOH+ 5.756e-007 5.345e-007 -6.240 -6.272 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.316e-008 1.317e-008 -7.881 -7.880 0.000

NaCO3- 8.050e-009 7.476e-009 -8.094 -8.126 -0.032

NaSO4- 3.742e-009 3.475e-009 -8.427 -8.459 -0.032

NaOH 1.610e-011 1.612e-011 -10.793 -10.793 0.000

O(0) 4.782e-004

O2 2.391e-004 2.394e-004 -3.621 -3.621 0.000

S(6) 1.154e-004

SO4-2 9.705e-005 7.255e-005 -4.013 -4.139 -0.126

CaSO4 1.130e-005 1.132e-005 -4.947 -4.946 0.000

MgSO4 7.011e-006 7.018e-006 -5.154 -5.154 0.000

NaSO4- 3.742e-009 3.475e-009 -8.427 -8.459 -0.032

KSO4- 1.838e-009 1.707e-009 -8.736 -8.768 -0.032

HSO4- 3.213e-011 2.984e-011 -10.493 -10.525 -0.032

CaHSO4+ 2.889e-013 2.683e-013 -12.539 -12.571 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.38 CaSO4

Aragonite 0.77 -7.59 -8.37 CaCO3

Calcite 0.92 -7.59 -8.51 CaCO3

CO2(g) -3.17 -4.69 -1.52 CO2

Dolomite 1.70 -15.50 -17.20 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.84 -28.01 -3.17 H2

H2O(g) -1.39 -0.00 1.39 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.70 -3.62 -2.93 O2

Initial solution 26. 29/8/2012 18:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.582e-004 4.582e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.420

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 324

Density (g/cm3) = 0.99592

Activity of water = 1.000

Ionic strength = 4.657e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.870e-003

Total CO2 (mol/kg) = 2.870e-003

Temperature (deg C) = 29.800

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551573e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.7988 0.7092

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 4.043e-006 3.752e-006 -5.393 -5.426 -0.032

H+ 4.066e-009 3.802e-009 -8.391 -8.420 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.870e-003

HCO3- 2.705e-003 2.517e-003 -2.568 -2.599 -0.031

CaCO3 4.721e-005 4.726e-005 -4.326 -4.326 0.000

CO3-2 4.534e-005 3.400e-005 -4.344 -4.469 -0.125

CaHCO3+ 2.749e-005 2.558e-005 -4.561 -4.592 -0.031

CO2 2.039e-005 2.041e-005 -4.691 -4.690 0.000

MgCO3 1.275e-005 1.277e-005 -4.894 -4.894 0.000

MgHCO3+ 1.187e-005 1.102e-005 -4.926 -4.958 -0.032

NaHCO3 1.312e-008 1.313e-008 -7.882 -7.882 0.000

NaCO3- 8.024e-009 7.453e-009 -8.096 -8.128 -0.032

Ca 1.081e-003

Ca+2 9.951e-004 7.458e-004 -3.002 -3.127 -0.125

CaCO3 4.721e-005 4.726e-005 -4.326 -4.326 0.000

CaHCO3+ 2.749e-005 2.558e-005 -4.561 -4.592 -0.031

CaSO4 1.128e-005 1.129e-005 -4.948 -4.947 0.000

CaOH+ 3.505e-008 3.255e-008 -7.455 -7.487 -0.032

CaHSO4+ 2.882e-013 2.677e-013 -12.540 -12.572 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.274 -0.032

H(0) 1.950e-028

H2 9.752e-029 9.763e-029 -28.011 -28.010 0.000

K 3.325e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.839e-009 1.708e-009 -8.735 -8.767 -0.032

KOH 2.810e-012 2.813e-012 -11.551 -11.551 0.000

Mg 5.184e-004

Mg+2 4.862e-004 3.656e-004 -3.313 -3.437 -0.124

MgCO3 1.275e-005 1.277e-005 -4.894 -4.894 0.000

MgHCO3+ 1.187e-005 1.102e-005 -4.926 -4.958 -0.032

MgSO4 7.018e-006 7.025e-006 -5.154 -5.153 0.000

MgOH+ 5.758e-007 5.348e-007 -6.240 -6.272 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.312e-008 1.313e-008 -7.882 -7.882 0.000

NaCO3- 8.024e-009 7.453e-009 -8.096 -8.128 -0.032

NaSO4- 3.744e-009 3.478e-009 -8.427 -8.459 -0.032

NaOH 1.610e-011 1.612e-011 -10.793 -10.793 0.000

O(0) 4.582e-004

O2 2.291e-004 2.294e-004 -3.640 -3.639 0.000

S(6) 1.154e-004

SO4-2 9.707e-005 7.259e-005 -4.013 -4.139 -0.126

CaSO4 1.128e-005 1.129e-005 -4.948 -4.947 0.000

MgSO4 7.018e-006 7.025e-006 -5.154 -5.153 0.000

NaSO4- 3.744e-009 3.478e-009 -8.427 -8.459 -0.032

KSO4- 1.839e-009 1.708e-009 -8.735 -8.767 -0.032

HSO4- 3.214e-011 2.985e-011 -10.493 -10.525 -0.032

CaHSO4+ 2.882e-013 2.677e-013 -12.540 -12.572 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.38 CaSO4

Aragonite 0.77 -7.60 -8.37 CaCO3

Calcite 0.91 -7.60 -8.51 CaCO3

CO2(g) -3.17 -4.69 -1.52 CO2

Dolomite 1.70 -15.50 -17.20 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.84 -28.01 -3.17 H2

H2O(g) -1.39 -0.00 1.39 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.71 -3.64 -2.93 O2

Initial solution 27. 29/8/2012 18:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.614e-004 4.614e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.430

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 323

Density (g/cm3) = 0.99595

Activity of water = 1.000

Ionic strength = 4.655e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.867e-003

Total CO2 (mol/kg) = 2.867e-003

Temperature (deg C) = 29.700

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551573e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.7976 0.7089

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 4.108e-006 3.812e-006 -5.386 -5.419 -0.032

H+ 3.973e-009 3.715e-009 -8.401 -8.430 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.867e-003

HCO3- 2.701e-003 2.513e-003 -2.569 -2.600 -0.031

CaCO3 4.801e-005 4.807e-005 -4.319 -4.318 0.000

CO3-2 4.624e-005 3.468e-005 -4.335 -4.460 -0.125

CaHCO3+ 2.740e-005 2.550e-005 -4.562 -4.593 -0.031

CO2 1.992e-005 1.994e-005 -4.701 -4.700 0.000

MgCO3 1.298e-005 1.300e-005 -4.887 -4.886 0.000

MgHCO3+ 1.184e-005 1.100e-005 -4.927 -4.959 -0.032

NaHCO3 1.310e-008 1.311e-008 -7.883 -7.882 0.000

NaCO3- 8.145e-009 7.565e-009 -8.089 -8.121 -0.032

Ca 1.081e-003

Ca+2 9.944e-004 7.453e-004 -3.002 -3.128 -0.125

CaCO3 4.801e-005 4.807e-005 -4.319 -4.318 0.000

CaHCO3+ 2.740e-005 2.550e-005 -4.562 -4.593 -0.031

CaSO4 1.126e-005 1.128e-005 -4.948 -4.948 0.000

CaOH+ 3.584e-008 3.329e-008 -7.446 -7.478 -0.032

CaHSO4+ 2.809e-013 2.609e-013 -12.551 -12.583 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.274 -0.032

H(0) 1.864e-028

H2 9.322e-029 9.332e-029 -28.030 -28.030 0.000

K 3.325e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.837e-009 1.706e-009 -8.736 -8.768 -0.032

KOH 2.875e-012 2.879e-012 -11.541 -11.541 0.000

Mg 5.184e-004

Mg+2 4.860e-004 3.654e-004 -3.313 -3.437 -0.124

MgCO3 1.298e-005 1.300e-005 -4.887 -4.886 0.000

MgHCO3+ 1.184e-005 1.100e-005 -4.927 -4.959 -0.032

MgSO4 7.001e-006 7.008e-006 -5.155 -5.154 0.000

MgOH+ 5.839e-007 5.423e-007 -6.234 -6.266 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.310e-008 1.311e-008 -7.883 -7.882 0.000

NaCO3- 8.145e-009 7.565e-009 -8.089 -8.121 -0.032

NaSO4- 3.743e-009 3.477e-009 -8.427 -8.459 -0.032

NaOH 1.648e-011 1.650e-011 -10.783 -10.783 0.000

O(0) 4.614e-004

O2 2.307e-004 2.309e-004 -3.637 -3.637 0.000

S(6) 1.154e-004

SO4-2 9.710e-005 7.262e-005 -4.013 -4.139 -0.126

CaSO4 1.126e-005 1.128e-005 -4.948 -4.948 0.000

MgSO4 7.001e-006 7.008e-006 -5.155 -5.154 0.000

NaSO4- 3.743e-009 3.477e-009 -8.427 -8.459 -0.032

KSO4- 1.837e-009 1.706e-009 -8.736 -8.768 -0.032

HSO4- 3.135e-011 2.912e-011 -10.504 -10.536 -0.032

CaHSO4+ 2.809e-013 2.609e-013 -12.551 -12.583 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.38 CaSO4

Aragonite 0.78 -7.59 -8.37 CaCO3

Calcite 0.92 -7.59 -8.51 CaCO3

CO2(g) -3.18 -4.70 -1.52 CO2

Dolomite 1.71 -15.48 -17.20 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.86 -28.03 -3.17 H2

H2O(g) -1.39 -0.00 1.39 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.71 -3.64 -2.92 O2

Initial solution 28. 29/8/2012 18:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.076e-004 5.076e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.400

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 323

Density (g/cm3) = 0.99598

Activity of water = 1.000

Ionic strength = 4.663e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.876e-003

Total CO2 (mol/kg) = 2.876e-003

Temperature (deg C) = 29.600

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551580e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8460 0.7116

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.806e-006 3.532e-006 -5.420 -5.452 -0.033

H+ 4.258e-009 3.981e-009 -8.371 -8.400 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.876e-003

HCO3- 2.714e-003 2.526e-003 -2.566 -2.598 -0.031

CaCO3 4.497e-005 4.502e-005 -4.347 -4.347 0.000

CO3-2 4.330e-005 3.247e-005 -4.363 -4.489 -0.125

CaHCO3+ 2.758e-005 2.566e-005 -4.559 -4.591 -0.031

CO2 2.147e-005 2.149e-005 -4.668 -4.668 0.000

MgCO3 1.216e-005 1.217e-005 -4.915 -4.915 0.000

MgHCO3+ 1.191e-005 1.106e-005 -4.924 -4.956 -0.032

NaHCO3 1.316e-008 1.318e-008 -7.881 -7.880 0.000

NaCO3- 7.589e-009 7.049e-009 -8.120 -8.152 -0.032

Ca 1.081e-003

Ca+2 9.973e-004 7.473e-004 -3.001 -3.126 -0.125

CaCO3 4.497e-005 4.502e-005 -4.347 -4.347 0.000

CaHCO3+ 2.758e-005 2.566e-005 -4.559 -4.591 -0.031

CaSO4 1.128e-005 1.129e-005 -4.948 -4.947 0.000

CaOH+ 3.354e-008 3.115e-008 -7.474 -7.507 -0.032

CaHSO4+ 3.011e-013 2.796e-013 -12.521 -12.553 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.274 -0.032

H(0) 2.143e-028

H2 1.071e-028 1.073e-028 -27.970 -27.970 0.000

K 3.325e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.833e-009 1.703e-009 -8.737 -8.769 -0.032

KOH 2.683e-012 2.686e-012 -11.571 -11.571 0.000

Mg 5.184e-004

Mg+2 4.868e-004 3.660e-004 -3.313 -3.437 -0.124

MgCO3 1.216e-005 1.217e-005 -4.915 -4.915 0.000

MgHCO3+ 1.191e-005 1.106e-005 -4.924 -4.956 -0.032

MgSO4 6.992e-006 6.999e-006 -5.155 -5.155 0.000

MgOH+ 5.410e-007 5.024e-007 -6.267 -6.299 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.316e-008 1.318e-008 -7.881 -7.880 0.000

NaCO3- 7.589e-009 7.049e-009 -8.120 -8.152 -0.032

NaSO4- 3.740e-009 3.474e-009 -8.427 -8.459 -0.032

NaOH 1.538e-011 1.540e-011 -10.813 -10.813 0.000

O(0) 5.076e-004

O2 2.538e-004 2.541e-004 -3.595 -3.595 0.000

S(6) 1.154e-004

SO4-2 9.709e-005 7.260e-005 -4.013 -4.139 -0.126

CaSO4 1.128e-005 1.129e-005 -4.948 -4.947 0.000

MgSO4 6.992e-006 6.999e-006 -5.155 -5.155 0.000

NaSO4- 3.740e-009 3.474e-009 -8.427 -8.459 -0.032

KSO4- 1.833e-009 1.703e-009 -8.737 -8.769 -0.032

HSO4- 3.351e-011 3.112e-011 -10.475 -10.507 -0.032

CaHSO4+ 3.011e-013 2.796e-013 -12.521 -12.553 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.38 CaSO4

Aragonite 0.75 -7.62 -8.37 CaCO3

Calcite 0.89 -7.62 -8.51 CaCO3

CO2(g) -3.15 -4.67 -1.52 CO2

Dolomite 1.65 -15.54 -17.20 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.80 -27.97 -3.17 H2

H2O(g) -1.39 -0.00 1.39 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.67 -3.60 -2.92 O2

Initial solution 29. 29/8/2012 18:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.864e-004 4.864e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.420

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 322

Density (g/cm3) = 0.99601

Activity of water = 1.000

Ionic strength = 4.659e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.871e-003

Total CO2 (mol/kg) = 2.871e-003

Temperature (deg C) = 29.500

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551576e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8294 0.7103

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.957e-006 3.671e-006 -5.403 -5.435 -0.032

H+ 4.066e-009 3.802e-009 -8.391 -8.420 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.871e-003

HCO3- 2.706e-003 2.519e-003 -2.568 -2.599 -0.031

CaCO3 4.670e-005 4.675e-005 -4.331 -4.330 0.000

CO3-2 4.512e-005 3.384e-005 -4.346 -4.471 -0.125

CaHCO3+ 2.743e-005 2.552e-005 -4.562 -4.593 -0.031

CO2 2.046e-005 2.048e-005 -4.689 -4.689 0.000

MgCO3 1.264e-005 1.265e-005 -4.898 -4.898 0.000

MgHCO3+ 1.186e-005 1.102e-005 -4.926 -4.958 -0.032

NaHCO3 1.313e-008 1.314e-008 -7.882 -7.881 0.000

NaCO3- 7.871e-009 7.311e-009 -8.104 -8.136 -0.032

Ca 1.081e-003

Ca+2 9.957e-004 7.463e-004 -3.002 -3.127 -0.125

CaCO3 4.670e-005 4.675e-005 -4.331 -4.330 0.000

CaHCO3+ 2.743e-005 2.552e-005 -4.562 -4.593 -0.031

CaSO4 1.126e-005 1.127e-005 -4.948 -4.948 0.000

CaOH+ 3.507e-008 3.257e-008 -7.455 -7.487 -0.032

CaHSO4+ 2.866e-013 2.662e-013 -12.543 -12.575 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.274 -0.032

H(0) 1.956e-028

H2 9.781e-029 9.791e-029 -28.010 -28.009 0.000

K 3.325e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.831e-009 1.701e-009 -8.737 -8.769 -0.032

KOH 2.810e-012 2.813e-012 -11.551 -11.551 0.000

Mg 5.184e-004

Mg+2 4.864e-004 3.657e-004 -3.313 -3.437 -0.124

MgCO3 1.264e-005 1.265e-005 -4.898 -4.898 0.000

MgHCO3+ 1.186e-005 1.102e-005 -4.926 -4.958 -0.032

MgSO4 6.973e-006 6.981e-006 -5.157 -5.156 0.000

MgOH+ 5.611e-007 5.212e-007 -6.251 -6.283 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.313e-008 1.314e-008 -7.882 -7.881 0.000

NaCO3- 7.871e-009 7.311e-009 -8.104 -8.136 -0.032

NaSO4- 3.740e-009 3.474e-009 -8.427 -8.459 -0.032

NaOH 1.610e-011 1.612e-011 -10.793 -10.793 0.000

O(0) 4.864e-004

O2 2.432e-004 2.434e-004 -3.614 -3.614 0.000

S(6) 1.154e-004

SO4-2 9.713e-005 7.264e-005 -4.013 -4.139 -0.126

CaSO4 1.126e-005 1.127e-005 -4.948 -4.948 0.000

MgSO4 6.973e-006 6.981e-006 -5.157 -5.156 0.000

NaSO4- 3.740e-009 3.474e-009 -8.427 -8.459 -0.032

KSO4- 1.831e-009 1.701e-009 -8.737 -8.769 -0.032

HSO4- 3.195e-011 2.967e-011 -10.496 -10.528 -0.032

CaHSO4+ 2.866e-013 2.662e-013 -12.543 -12.575 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.38 CaSO4

Aragonite 0.77 -7.60 -8.37 CaCO3

Calcite 0.91 -7.60 -8.51 CaCO3

CO2(g) -3.17 -4.69 -1.52 CO2

Dolomite 1.69 -15.51 -17.19 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.84 -28.01 -3.17 H2

H2O(g) -1.40 -0.00 1.40 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.69 -3.61 -2.92 O2

Initial solution 30. 29/8/2012 19:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.908e-004 4.908e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.420

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 321

Density (g/cm3) = 0.99604

Activity of water = 1.000

Ionic strength = 4.660e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.871e-003

Total CO2 (mol/kg) = 2.871e-003

Temperature (deg C) = 29.400

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551577e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8384 0.7106

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.928e-006 3.645e-006 -5.406 -5.438 -0.032

H+ 4.066e-009 3.802e-009 -8.391 -8.420 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.871e-003

HCO3- 2.707e-003 2.519e-003 -2.568 -2.599 -0.031

CaCO3 4.653e-005 4.658e-005 -4.332 -4.332 0.000

CO3-2 4.505e-005 3.379e-005 -4.346 -4.471 -0.125

CaHCO3+ 2.740e-005 2.550e-005 -4.562 -4.593 -0.031

CO2 2.049e-005 2.051e-005 -4.689 -4.688 0.000

MgCO3 1.260e-005 1.262e-005 -4.900 -4.899 0.000

MgHCO3+ 1.186e-005 1.102e-005 -4.926 -4.958 -0.032

NaHCO3 1.313e-008 1.314e-008 -7.882 -7.881 0.000

NaCO3- 7.820e-009 7.264e-009 -8.107 -8.139 -0.032

Ca 1.081e-003

Ca+2 9.959e-004 7.464e-004 -3.002 -3.127 -0.125

CaCO3 4.653e-005 4.658e-005 -4.332 -4.332 0.000

CaHCO3+ 2.740e-005 2.550e-005 -4.562 -4.593 -0.031

CaSO4 1.126e-005 1.127e-005 -4.949 -4.948 0.000

CaOH+ 3.508e-008 3.258e-008 -7.455 -7.487 -0.032

CaHSO4+ 2.861e-013 2.657e-013 -12.543 -12.576 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.316e-005 -4.242 -4.274 -0.032

H(0) 1.958e-028

H2 9.790e-029 9.801e-029 -28.009 -28.009 0.000

K 3.325e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.829e-009 1.698e-009 -8.738 -8.770 -0.032

KOH 2.810e-012 2.813e-012 -11.551 -11.551 0.000

Mg 5.184e-004

Mg+2 4.864e-004 3.658e-004 -3.313 -3.437 -0.124

MgCO3 1.260e-005 1.262e-005 -4.900 -4.899 0.000

MgHCO3+ 1.186e-005 1.102e-005 -4.926 -4.958 -0.032

MgSO4 6.959e-006 6.966e-006 -5.157 -5.157 0.000

MgOH+ 5.563e-007 5.167e-007 -6.255 -6.287 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.278e-006 -5.001 -5.033 -0.032

NaHCO3 1.313e-008 1.314e-008 -7.882 -7.881 0.000

NaCO3- 7.820e-009 7.264e-009 -8.107 -8.139 -0.032

NaSO4- 3.739e-009 3.472e-009 -8.427 -8.459 -0.032

NaOH 1.610e-011 1.612e-011 -10.793 -10.793 0.000

O(0) 4.908e-004

O2 2.454e-004 2.456e-004 -3.610 -3.610 0.000

S(6) 1.154e-004

SO4-2 9.715e-005 7.266e-005 -4.013 -4.139 -0.126

CaSO4 1.126e-005 1.127e-005 -4.949 -4.948 0.000

MgSO4 6.959e-006 6.966e-006 -5.157 -5.157 0.000

NaSO4- 3.739e-009 3.472e-009 -8.427 -8.459 -0.032

KSO4- 1.829e-009 1.698e-009 -8.738 -8.770 -0.032

HSO4- 3.188e-011 2.961e-011 -10.496 -10.529 -0.032

CaHSO4+ 2.861e-013 2.657e-013 -12.543 -12.576 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.38 CaSO4

Aragonite 0.77 -7.60 -8.37 CaCO3

Calcite 0.91 -7.60 -8.51 CaCO3

CO2(g) -3.17 -4.69 -1.52 CO2

Dolomite 1.68 -15.51 -17.19 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.84 -28.01 -3.17 H2

H2O(g) -1.40 -0.00 1.40 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.69 -3.61 -2.92 O2

Initial solution 31. 29/8/2012 19:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.949e-003 2.949e-003

Ca 1.077e-003 1.077e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.864e-004 4.864e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.420

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 320

Density (g/cm3) = 0.99607

Activity of water = 1.000

Ionic strength = 4.649e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.861e-003

Total CO2 (mol/kg) = 2.861e-003

Temperature (deg C) = 29.300

Electrical balance (eq) = -3.183e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.53

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551573e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8455 0.7108

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.899e-006 3.619e-006 -5.409 -5.441 -0.032

H+ 4.065e-009 3.802e-009 -8.391 -8.420 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.861e-003

HCO3- 2.698e-003 2.511e-003 -2.569 -2.600 -0.031

CaCO3 4.607e-005 4.612e-005 -4.337 -4.336 0.000

CO3-2 4.482e-005 3.362e-005 -4.349 -4.473 -0.125

CaHCO3+ 2.721e-005 2.532e-005 -4.565 -4.597 -0.031

CO2 2.044e-005 2.047e-005 -4.689 -4.689 0.000

MgCO3 1.253e-005 1.254e-005 -4.902 -4.902 0.000

MgHCO3+ 1.182e-005 1.098e-005 -4.927 -4.959 -0.032

NaHCO3 1.309e-008 1.310e-008 -7.883 -7.883 0.000

NaCO3- 7.744e-009 7.193e-009 -8.111 -8.143 -0.032

Ca 1.077e-003

Ca+2 9.928e-004 7.444e-004 -3.003 -3.128 -0.125

CaCO3 4.607e-005 4.612e-005 -4.337 -4.336 0.000

CaHCO3+ 2.721e-005 2.532e-005 -4.565 -4.597 -0.031

CaSO4 1.122e-005 1.124e-005 -4.950 -4.949 0.000

CaOH+ 3.498e-008 3.249e-008 -7.456 -7.488 -0.032

CaHSO4+ 2.849e-013 2.646e-013 -12.545 -12.577 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.316e-005 -4.242 -4.274 -0.032

H(0) 1.960e-028

H2 9.800e-029 9.810e-029 -28.009 -28.008 0.000

K 3.325e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.827e-009 1.697e-009 -8.738 -8.770 -0.032

KOH 2.810e-012 2.813e-012 -11.551 -11.551 0.000

Mg 5.184e-004

Mg+2 4.865e-004 3.660e-004 -3.313 -3.437 -0.124

MgCO3 1.253e-005 1.254e-005 -4.902 -4.902 0.000

MgHCO3+ 1.182e-005 1.098e-005 -4.927 -4.959 -0.032

MgSO4 6.951e-006 6.958e-006 -5.158 -5.158 0.000

MgOH+ 5.517e-007 5.125e-007 -6.258 -6.290 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.279e-006 -5.001 -5.033 -0.032

NaHCO3 1.309e-008 1.310e-008 -7.883 -7.883 0.000

NaCO3- 7.744e-009 7.193e-009 -8.111 -8.143 -0.032

NaSO4- 3.739e-009 3.473e-009 -8.427 -8.459 -0.032

NaOH 1.611e-011 1.612e-011 -10.793 -10.793 0.000

O(0) 4.864e-004

O2 2.432e-004 2.434e-004 -3.614 -3.614 0.000

S(6) 1.154e-004

SO4-2 9.719e-005 7.271e-005 -4.012 -4.138 -0.126

CaSO4 1.122e-005 1.124e-005 -4.950 -4.949 0.000

MgSO4 6.951e-006 6.958e-006 -5.158 -5.158 0.000

NaSO4- 3.739e-009 3.473e-009 -8.427 -8.459 -0.032

KSO4- 1.827e-009 1.697e-009 -8.738 -8.770 -0.032

HSO4- 3.183e-011 2.957e-011 -10.497 -10.529 -0.032

CaHSO4+ 2.849e-013 2.646e-013 -12.545 -12.577 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.38 CaSO4

Aragonite 0.76 -7.60 -8.36 CaCO3

Calcite 0.90 -7.60 -8.51 CaCO3

CO2(g) -3.17 -4.69 -1.52 CO2

Dolomite 1.68 -15.51 -17.19 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.84 -28.01 -3.17 H2

H2O(g) -1.40 -0.00 1.40 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.69 -3.61 -2.92 O2

Initial solution 32. 29/8/2012 19:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.726e-004 4.726e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.400

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 321

Density (g/cm3) = 0.99610

Activity of water = 1.000

Ionic strength = 4.666e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.877e-003

Total CO2 (mol/kg) = 2.877e-003

Temperature (deg C) = 29.200

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551576e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8704 0.7121

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.698e-006 3.431e-006 -5.432 -5.465 -0.032

H+ 4.257e-009 3.981e-009 -8.371 -8.400 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.877e-003

HCO3- 2.717e-003 2.528e-003 -2.566 -2.597 -0.031

CaCO3 4.432e-005 4.437e-005 -4.353 -4.353 0.000

CO3-2 4.303e-005 3.227e-005 -4.366 -4.491 -0.125

CaHCO3+ 2.749e-005 2.558e-005 -4.561 -4.592 -0.031

CO2 2.157e-005 2.160e-005 -4.666 -4.666 0.000

MgCO3 1.201e-005 1.203e-005 -4.920 -4.920 0.000

MgHCO3+ 1.190e-005 1.106e-005 -4.924 -4.956 -0.032

NaHCO3 1.318e-008 1.319e-008 -7.880 -7.880 0.000

NaCO3- 7.396e-009 6.869e-009 -8.131 -8.163 -0.032

Ca 1.081e-003

Ca+2 9.980e-004 7.480e-004 -3.001 -3.126 -0.125

CaCO3 4.432e-005 4.437e-005 -4.353 -4.353 0.000

CaHCO3+ 2.749e-005 2.558e-005 -4.561 -4.592 -0.031

CaSO4 1.126e-005 1.127e-005 -4.948 -4.948 0.000

CaOH+ 3.357e-008 3.118e-008 -7.474 -7.506 -0.032

CaHSO4+ 2.989e-013 2.776e-013 -12.524 -12.557 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.274 -0.032

H(0) 2.151e-028

H2 1.076e-028 1.077e-028 -27.968 -27.968 0.000

K 3.325e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.823e-009 1.693e-009 -8.739 -8.771 -0.032

KOH 2.683e-012 2.686e-012 -11.571 -11.571 0.000

Mg 5.184e-004

Mg+2 4.870e-004 3.662e-004 -3.312 -3.436 -0.124

MgCO3 1.201e-005 1.203e-005 -4.920 -4.920 0.000

MgHCO3+ 1.190e-005 1.106e-005 -4.924 -4.956 -0.032

MgSO4 6.933e-006 6.940e-006 -5.159 -5.159 0.000

MgOH+ 5.226e-007 4.854e-007 -6.282 -6.314 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.278e-006 -5.001 -5.033 -0.032

NaHCO3 1.318e-008 1.319e-008 -7.880 -7.880 0.000

NaCO3- 7.396e-009 6.869e-009 -8.131 -8.163 -0.032

NaSO4- 3.735e-009 3.469e-009 -8.428 -8.460 -0.032

NaOH 1.538e-011 1.540e-011 -10.813 -10.813 0.000

O(0) 4.726e-004

O2 2.363e-004 2.366e-004 -3.627 -3.626 0.000

S(6) 1.154e-004

SO4-2 9.717e-005 7.267e-005 -4.012 -4.139 -0.126

CaSO4 1.126e-005 1.127e-005 -4.948 -4.948 0.000

MgSO4 6.933e-006 6.940e-006 -5.159 -5.159 0.000

NaSO4- 3.735e-009 3.469e-009 -8.428 -8.460 -0.032

KSO4- 1.823e-009 1.693e-009 -8.739 -8.771 -0.032

HSO4- 3.324e-011 3.087e-011 -10.478 -10.510 -0.032

CaHSO4+ 2.989e-013 2.776e-013 -12.524 -12.557 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.75 -7.62 -8.36 CaCO3

Calcite 0.89 -7.62 -8.50 CaCO3

CO2(g) -3.15 -4.67 -1.52 CO2

Dolomite 1.64 -15.54 -17.19 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.80 -27.97 -3.17 H2

H2O(g) -1.40 -0.00 1.40 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.70 -3.63 -2.92 O2

Initial solution 33. 29/8/2012 19:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.949e-003 2.949e-003

Ca 1.077e-003 1.077e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.789e-004 4.789e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.400

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 320

Density (g/cm3) = 0.99610

Activity of water = 1.000

Ionic strength = 4.655e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.867e-003

Total CO2 (mol/kg) = 2.867e-003

Temperature (deg C) = 29.200

Electrical balance (eq) = -3.183e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.52

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551574e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8718 0.7122

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.697e-006 3.431e-006 -5.432 -5.465 -0.032

H+ 4.257e-009 3.981e-009 -8.371 -8.400 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.867e-003

HCO3- 2.707e-003 2.520e-003 -2.567 -2.599 -0.031

CaCO3 4.404e-005 4.409e-005 -4.356 -4.356 0.000

CO3-2 4.287e-005 3.216e-005 -4.368 -4.493 -0.125

CaHCO3+ 2.731e-005 2.542e-005 -4.564 -4.595 -0.031

CO2 2.150e-005 2.152e-005 -4.668 -4.667 0.000

MgCO3 1.198e-005 1.199e-005 -4.922 -4.921 0.000

MgHCO3+ 1.187e-005 1.102e-005 -4.926 -4.958 -0.032

NaHCO3 1.313e-008 1.315e-008 -7.882 -7.881 0.000

NaCO3- 7.371e-009 6.847e-009 -8.132 -8.165 -0.032

Ca 1.077e-003

Ca+2 9.947e-004 7.458e-004 -3.002 -3.127 -0.125

CaCO3 4.404e-005 4.409e-005 -4.356 -4.356 0.000

CaHCO3+ 2.731e-005 2.542e-005 -4.564 -4.595 -0.031

CaSO4 1.123e-005 1.125e-005 -4.950 -4.949 0.000

CaOH+ 3.347e-008 3.109e-008 -7.475 -7.507 -0.032

CaHSO4+ 2.982e-013 2.770e-013 -12.526 -12.558 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.316e-005 -4.242 -4.274 -0.032

H(0) 2.151e-028

H2 1.076e-028 1.077e-028 -27.968 -27.968 0.000

K 3.325e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.824e-009 1.694e-009 -8.739 -8.771 -0.032

KOH 2.684e-012 2.687e-012 -11.571 -11.571 0.000

Mg 5.184e-004

Mg+2 4.871e-004 3.664e-004 -3.312 -3.436 -0.124

MgCO3 1.198e-005 1.199e-005 -4.922 -4.921 0.000

MgHCO3+ 1.187e-005 1.102e-005 -4.926 -4.958 -0.032

MgSO4 6.940e-006 6.947e-006 -5.159 -5.158 0.000

MgOH+ 5.228e-007 4.856e-007 -6.282 -6.314 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.279e-006 -5.001 -5.033 -0.032

NaHCO3 1.313e-008 1.315e-008 -7.882 -7.881 0.000

NaCO3- 7.371e-009 6.847e-009 -8.132 -8.165 -0.032

NaSO4- 3.737e-009 3.471e-009 -8.428 -8.460 -0.032

NaOH 1.538e-011 1.540e-011 -10.813 -10.813 0.000

O(0) 4.789e-004

O2 2.394e-004 2.397e-004 -3.621 -3.620 0.000

S(6) 1.154e-004

SO4-2 9.719e-005 7.270e-005 -4.012 -4.138 -0.126

CaSO4 1.123e-005 1.125e-005 -4.950 -4.949 0.000

MgSO4 6.940e-006 6.947e-006 -5.159 -5.158 0.000

NaSO4- 3.737e-009 3.471e-009 -8.428 -8.460 -0.032

KSO4- 1.824e-009 1.694e-009 -8.739 -8.771 -0.032

HSO4- 3.325e-011 3.089e-011 -10.478 -10.510 -0.032

CaHSO4+ 2.982e-013 2.770e-013 -12.526 -12.558 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.38 CaSO4

Aragonite 0.74 -7.62 -8.36 CaCO3

Calcite 0.88 -7.62 -8.50 CaCO3

CO2(g) -3.15 -4.67 -1.52 CO2

Dolomite 1.64 -15.55 -17.19 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.80 -27.97 -3.17 H2

H2O(g) -1.40 -0.00 1.40 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.70 -3.62 -2.92 O2

Initial solution 34. 29/8/2012 20:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.990e-003 2.990e-003

Ca 1.092e-003 1.092e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.620e-004 4.620e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.390

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 322

Density (g/cm3) = 0.99613

Activity of water = 1.000

Ionic strength = 4.703e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.910e-003

Total CO2 (mol/kg) = 2.910e-003

Temperature (deg C) = 29.100

Electrical balance (eq) = -4.336e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.71

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551585e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8860 0.7128

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.588e-006 3.329e-006 -5.445 -5.478 -0.033

H+ 4.358e-009 4.074e-009 -8.361 -8.390 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.910e-003

HCO3- 2.749e-003 2.558e-003 -2.561 -2.592 -0.031

CaCO3 4.407e-005 4.412e-005 -4.356 -4.355 0.000

CO3-2 4.250e-005 3.184e-005 -4.372 -4.497 -0.125

CaHCO3+ 2.806e-005 2.610e-005 -4.552 -4.583 -0.031

CO2 2.236e-005 2.238e-005 -4.651 -4.650 0.000

MgHCO3+ 1.203e-005 1.117e-005 -4.920 -4.952 -0.032

MgCO3 1.183e-005 1.184e-005 -4.927 -4.927 0.000

NaHCO3 1.333e-008 1.334e-008 -7.875 -7.875 0.000

NaCO3- 7.263e-009 6.744e-009 -8.139 -8.171 -0.032

Ca 1.092e-003

Ca+2 1.009e-003 7.554e-004 -2.996 -3.122 -0.126

CaCO3 4.407e-005 4.412e-005 -4.356 -4.355 0.000

CaHCO3+ 2.806e-005 2.610e-005 -4.552 -4.583 -0.031

CaSO4 1.134e-005 1.136e-005 -4.945 -4.945 0.000

CaOH+ 3.314e-008 3.077e-008 -7.480 -7.512 -0.032

CaHSO4+ 3.078e-013 2.858e-013 -12.512 -12.544 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 2.255e-028

H2 1.127e-028 1.129e-028 -27.948 -27.947 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.817e-009 1.687e-009 -8.741 -8.773 -0.032

KOH 2.622e-012 2.625e-012 -11.581 -11.581 0.000

Mg 5.184e-004

Mg+2 4.871e-004 3.659e-004 -3.312 -3.437 -0.124

MgHCO3+ 1.203e-005 1.117e-005 -4.920 -4.952 -0.032

MgCO3 1.183e-005 1.184e-005 -4.927 -4.927 0.000

MgSO4 6.900e-006 6.908e-006 -5.161 -5.161 0.000

MgOH+ 5.060e-007 4.699e-007 -6.296 -6.328 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.333e-008 1.334e-008 -7.875 -7.875 0.000

NaCO3- 7.263e-009 6.744e-009 -8.139 -8.171 -0.032

NaSO4- 3.727e-009 3.461e-009 -8.429 -8.461 -0.032

NaOH 1.503e-011 1.504e-011 -10.823 -10.823 0.000

O(0) 4.620e-004

O2 2.310e-004 2.312e-004 -3.636 -3.636 0.000

S(6) 1.154e-004

SO4-2 9.712e-005 7.256e-005 -4.013 -4.139 -0.127

CaSO4 1.134e-005 1.136e-005 -4.945 -4.945 0.000

MgSO4 6.900e-006 6.908e-006 -5.161 -5.161 0.000

NaSO4- 3.727e-009 3.461e-009 -8.429 -8.461 -0.032

KSO4- 1.817e-009 1.687e-009 -8.741 -8.773 -0.032

HSO4- 3.389e-011 3.147e-011 -10.470 -10.502 -0.032

CaHSO4+ 3.078e-013 2.858e-013 -12.512 -12.544 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.74 -7.62 -8.36 CaCO3

Calcite 0.89 -7.62 -8.50 CaCO3

CO2(g) -3.14 -4.65 -1.51 CO2

Dolomite 1.63 -15.55 -17.18 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.78 -27.95 -3.17 H2

H2O(g) -1.41 -0.00 1.41 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.72 -3.64 -2.92 O2

Initial solution 35. 29/8/2012 20:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.980e-003 2.980e-003

Ca 1.089e-003 1.089e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.958e-004 4.958e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.380

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 321

Density (g/cm3) = 0.99616

Activity of water = 1.000

Ionic strength = 4.695e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.903e-003

Total CO2 (mol/kg) = 2.903e-003

Temperature (deg C) = 29.000

Electrical balance (eq) = -4.035e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.66

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551586e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9117 0.7141

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.481e-006 3.229e-006 -5.458 -5.491 -0.033

H+ 4.459e-009 4.169e-009 -8.351 -8.380 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.903e-003

HCO3- 2.744e-003 2.553e-003 -2.562 -2.593 -0.031

CaCO3 4.274e-005 4.279e-005 -4.369 -4.369 0.000

CO3-2 4.138e-005 3.101e-005 -4.383 -4.509 -0.125

CaHCO3+ 2.792e-005 2.597e-005 -4.554 -4.585 -0.031

CO2 2.286e-005 2.289e-005 -4.641 -4.640 0.000

MgHCO3+ 1.202e-005 1.116e-005 -4.920 -4.952 -0.032

MgCO3 1.151e-005 1.153e-005 -4.939 -4.938 0.000

NaHCO3 1.331e-008 1.332e-008 -7.876 -7.875 0.000

NaCO3- 7.039e-009 6.536e-009 -8.153 -8.185 -0.032

Ca 1.089e-003

Ca+2 1.007e-003 7.539e-004 -2.997 -3.123 -0.126

CaCO3 4.274e-005 4.279e-005 -4.369 -4.369 0.000

CaHCO3+ 2.792e-005 2.597e-005 -4.554 -4.585 -0.031

CaSO4 1.132e-005 1.133e-005 -4.946 -4.946 0.000

CaOH+ 3.232e-008 3.001e-008 -7.491 -7.523 -0.032

CaHSO4+ 3.138e-013 2.914e-013 -12.503 -12.535 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 2.363e-028

H2 1.182e-028 1.183e-028 -27.928 -27.927 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.815e-009 1.685e-009 -8.741 -8.773 -0.032

KOH 2.562e-012 2.565e-012 -11.591 -11.591 0.000

Mg 5.184e-004

Mg+2 4.875e-004 3.663e-004 -3.312 -3.436 -0.124

MgHCO3+ 1.202e-005 1.116e-005 -4.920 -4.952 -0.032

MgCO3 1.151e-005 1.153e-005 -4.939 -4.938 0.000

MgSO4 6.894e-006 6.901e-006 -5.162 -5.161 0.000

MgOH+ 4.906e-007 4.556e-007 -6.309 -6.341 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.331e-008 1.332e-008 -7.876 -7.875 0.000

NaCO3- 7.039e-009 6.536e-009 -8.153 -8.185 -0.032

NaSO4- 3.727e-009 3.461e-009 -8.429 -8.461 -0.032

NaOH 1.468e-011 1.470e-011 -10.833 -10.833 0.000

O(0) 4.958e-004

O2 2.479e-004 2.481e-004 -3.606 -3.605 0.000

S(6) 1.154e-004

SO4-2 9.715e-005 7.260e-005 -4.013 -4.139 -0.127

CaSO4 1.132e-005 1.133e-005 -4.946 -4.946 0.000

MgSO4 6.894e-006 6.901e-006 -5.162 -5.161 0.000

NaSO4- 3.727e-009 3.461e-009 -8.429 -8.461 -0.032

KSO4- 1.815e-009 1.685e-009 -8.741 -8.773 -0.032

HSO4- 3.463e-011 3.215e-011 -10.461 -10.493 -0.032

CaHSO4+ 3.138e-013 2.914e-013 -12.503 -12.535 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.73 -7.63 -8.36 CaCO3

Calcite 0.87 -7.63 -8.50 CaCO3

CO2(g) -3.13 -4.64 -1.51 CO2

Dolomite 1.61 -15.58 -17.18 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.76 -27.93 -3.17 H2

H2O(g) -1.41 -0.00 1.41 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.69 -3.61 -2.92 O2

Initial solution 36. 29/8/2012 20:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.176e-004 5.176e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.390

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 322

Density (g/cm3) = 0.99619

Activity of water = 1.000

Ionic strength = 4.716e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.920e-003

Total CO2 (mol/kg) = 2.920e-003

Temperature (deg C) = 28.900

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.75

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551594e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9145 0.7140

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.537e-006 3.281e-006 -5.451 -5.484 -0.033

H+ 4.358e-009 4.074e-009 -8.361 -8.390 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.920e-003

HCO3- 2.759e-003 2.567e-003 -2.559 -2.591 -0.031

CaCO3 4.402e-005 4.407e-005 -4.356 -4.356 0.000

CO3-2 4.251e-005 3.184e-005 -4.371 -4.497 -0.126

CaHCO3+ 2.818e-005 2.622e-005 -4.550 -4.581 -0.031

CO2 2.248e-005 2.251e-005 -4.648 -4.648 0.000

MgHCO3+ 1.206e-005 1.120e-005 -4.919 -4.951 -0.032

MgCO3 1.179e-005 1.180e-005 -4.928 -4.928 0.000

NaHCO3 1.337e-008 1.339e-008 -7.874 -7.873 0.000

NaCO3- 7.192e-009 6.678e-009 -8.143 -8.175 -0.032

Ca 1.096e-003

Ca+2 1.012e-003 7.579e-004 -2.995 -3.120 -0.126

CaCO3 4.402e-005 4.407e-005 -4.356 -4.356 0.000

CaHCO3+ 2.818e-005 2.622e-005 -4.550 -4.581 -0.031

CaSO4 1.136e-005 1.137e-005 -4.945 -4.944 0.000

CaOH+ 3.325e-008 3.087e-008 -7.478 -7.510 -0.032

CaHSO4+ 3.075e-013 2.855e-013 -12.512 -12.544 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 2.259e-028

H2 1.129e-028 1.131e-028 -27.947 -27.947 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.811e-009 1.681e-009 -8.742 -8.774 -0.032

KOH 2.622e-012 2.624e-012 -11.581 -11.581 0.000

Mg 5.184e-004

Mg+2 4.872e-004 3.659e-004 -3.312 -3.437 -0.124

MgHCO3+ 1.206e-005 1.120e-005 -4.919 -4.951 -0.032

MgCO3 1.179e-005 1.180e-005 -4.928 -4.928 0.000

MgSO4 6.864e-006 6.872e-006 -5.163 -5.163 0.000

MgOH+ 4.972e-007 4.616e-007 -6.303 -6.336 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.337e-008 1.339e-008 -7.874 -7.873 0.000

NaCO3- 7.192e-009 6.678e-009 -8.143 -8.175 -0.032

NaSO4- 3.722e-009 3.456e-009 -8.429 -8.461 -0.032

NaOH 1.502e-011 1.504e-011 -10.823 -10.823 0.000

O(0) 5.176e-004

O2 2.588e-004 2.591e-004 -3.587 -3.587 0.000

S(6) 1.154e-004

SO4-2 9.714e-005 7.255e-005 -4.013 -4.139 -0.127

CaSO4 1.136e-005 1.137e-005 -4.945 -4.944 0.000

MgSO4 6.864e-006 6.872e-006 -5.163 -5.163 0.000

NaSO4- 3.722e-009 3.456e-009 -8.429 -8.461 -0.032

KSO4- 1.811e-009 1.681e-009 -8.742 -8.774 -0.032

HSO4- 3.374e-011 3.133e-011 -10.472 -10.504 -0.032

CaHSO4+ 3.075e-013 2.855e-013 -12.512 -12.544 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.74 -7.62 -8.36 CaCO3

Calcite 0.89 -7.62 -8.50 CaCO3

CO2(g) -3.14 -4.65 -1.51 CO2

Dolomite 1.63 -15.55 -17.18 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.78 -27.95 -3.17 H2

H2O(g) -1.41 -0.00 1.41 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.67 -3.59 -2.92 O2

Initial solution 37. 29/8/2012 20:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.564e-004 4.564e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.360

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 322

Density (g/cm3) = 0.99622

Activity of water = 1.000

Ionic strength = 4.723e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.929e-003

Total CO2 (mol/kg) = 2.929e-003

Temperature (deg C) = 28.800

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.75

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551590e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9389 0.7153

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.277e-006 3.040e-006 -5.485 -5.517 -0.033

H+ 4.670e-009 4.365e-009 -8.331 -8.360 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.929e-003

HCO3- 2.772e-003 2.579e-003 -2.557 -2.589 -0.031

CaCO3 4.120e-005 4.125e-005 -4.385 -4.385 0.000

CO3-2 3.979e-005 2.980e-005 -4.400 -4.526 -0.126

CaHCO3+ 2.834e-005 2.637e-005 -4.548 -4.579 -0.031

CO2 2.422e-005 2.425e-005 -4.616 -4.615 0.000

MgHCO3+ 1.213e-005 1.126e-005 -4.916 -4.948 -0.032

MgCO3 1.103e-005 1.104e-005 -4.957 -4.957 0.000

NaHCO3 1.343e-008 1.345e-008 -7.872 -7.871 0.000

NaCO3- 6.698e-009 6.218e-009 -8.174 -8.206 -0.032

Ca 1.096e-003

Ca+2 1.015e-003 7.598e-004 -2.993 -3.119 -0.126

CaCO3 4.120e-005 4.125e-005 -4.385 -4.385 0.000

CaHCO3+ 2.834e-005 2.637e-005 -4.548 -4.579 -0.031

CaSO4 1.138e-005 1.139e-005 -4.944 -4.944 0.000

CaOH+ 3.111e-008 2.888e-008 -7.507 -7.539 -0.032

CaHSO4+ 3.295e-013 3.059e-013 -12.482 -12.514 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 2.596e-028

H2 1.298e-028 1.299e-028 -27.887 -27.886 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.807e-009 1.678e-009 -8.743 -8.775 -0.032

KOH 2.446e-012 2.449e-012 -11.611 -11.611 0.000

Mg 5.184e-004

Mg+2 4.879e-004 3.664e-004 -3.312 -3.436 -0.124

MgHCO3+ 1.213e-005 1.126e-005 -4.916 -4.948 -0.032

MgCO3 1.103e-005 1.104e-005 -4.957 -4.957 0.000

MgSO4 6.855e-006 6.862e-006 -5.164 -5.164 0.000

MgOH+ 4.606e-007 4.276e-007 -6.337 -6.369 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.343e-008 1.345e-008 -7.872 -7.871 0.000

NaCO3- 6.698e-009 6.218e-009 -8.174 -8.206 -0.032

NaSO4- 3.719e-009 3.453e-009 -8.430 -8.462 -0.032

NaOH 1.402e-011 1.404e-011 -10.853 -10.853 0.000

O(0) 4.564e-004

O2 2.282e-004 2.284e-004 -3.642 -3.641 0.000

S(6) 1.154e-004

SO4-2 9.713e-005 7.254e-005 -4.013 -4.139 -0.127

CaSO4 1.138e-005 1.139e-005 -4.944 -4.944 0.000

MgSO4 6.855e-006 6.862e-006 -5.164 -5.164 0.000

NaSO4- 3.719e-009 3.453e-009 -8.430 -8.462 -0.032

KSO4- 1.807e-009 1.678e-009 -8.743 -8.775 -0.032

HSO4- 3.607e-011 3.349e-011 -10.443 -10.475 -0.032

CaHSO4+ 3.295e-013 3.059e-013 -12.482 -12.514 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.72 -7.65 -8.36 CaCO3

Calcite 0.86 -7.65 -8.50 CaCO3

CO2(g) -3.10 -4.62 -1.51 CO2

Dolomite 1.57 -15.61 -17.18 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.72 -27.89 -3.17 H2

H2O(g) -1.41 -0.00 1.41 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.72 -3.64 -2.92 O2

Initial solution 38. 29/8/2012 21:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.501e-004 4.501e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.370

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 322

Density (g/cm3) = 0.99622

Activity of water = 1.000

Ionic strength = 4.721e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.926e-003

Total CO2 (mol/kg) = 2.926e-003

Temperature (deg C) = 28.800

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.75

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551589e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9274 0.7146

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.353e-006 3.110e-006 -5.475 -5.507 -0.033

H+ 4.563e-009 4.266e-009 -8.341 -8.370 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.926e-003

HCO3- 2.768e-003 2.575e-003 -2.558 -2.589 -0.031

CaCO3 4.207e-005 4.212e-005 -4.376 -4.376 0.000

CO3-2 4.066e-005 3.045e-005 -4.391 -4.516 -0.126

CaHCO3+ 2.828e-005 2.631e-005 -4.548 -4.580 -0.031

CO2 2.364e-005 2.367e-005 -4.626 -4.626 0.000

MgHCO3+ 1.211e-005 1.124e-005 -4.917 -4.949 -0.032

MgCO3 1.127e-005 1.128e-005 -4.948 -4.948 0.000

NaHCO3 1.342e-008 1.343e-008 -7.872 -7.872 0.000

NaCO3- 6.844e-009 6.354e-009 -8.165 -8.197 -0.032

Ca 1.096e-003

Ca+2 1.014e-003 7.592e-004 -2.994 -3.120 -0.126

CaCO3 4.207e-005 4.212e-005 -4.376 -4.376 0.000

CaHCO3+ 2.828e-005 2.631e-005 -4.548 -4.580 -0.031

CaSO4 1.137e-005 1.138e-005 -4.944 -4.944 0.000

CaOH+ 3.181e-008 2.953e-008 -7.497 -7.530 -0.032

CaHSO4+ 3.218e-013 2.988e-013 -12.492 -12.525 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 2.479e-028

H2 1.240e-028 1.241e-028 -27.907 -27.906 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.807e-009 1.678e-009 -8.743 -8.775 -0.032

KOH 2.503e-012 2.506e-012 -11.601 -11.601 0.000

Mg 5.184e-004

Mg+2 4.877e-004 3.662e-004 -3.312 -3.436 -0.124

MgHCO3+ 1.211e-005 1.124e-005 -4.917 -4.949 -0.032

MgCO3 1.127e-005 1.128e-005 -4.948 -4.948 0.000

MgSO4 6.853e-006 6.861e-006 -5.164 -5.164 0.000

MgOH+ 4.711e-007 4.374e-007 -6.327 -6.359 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.342e-008 1.343e-008 -7.872 -7.872 0.000

NaCO3- 6.844e-009 6.354e-009 -8.165 -8.197 -0.032

NaSO4- 3.720e-009 3.454e-009 -8.430 -8.462 -0.032

NaOH 1.435e-011 1.436e-011 -10.843 -10.843 0.000

O(0) 4.501e-004

O2 2.251e-004 2.253e-004 -3.648 -3.647 0.000

S(6) 1.154e-004

SO4-2 9.714e-005 7.255e-005 -4.013 -4.139 -0.127

CaSO4 1.137e-005 1.138e-005 -4.944 -4.944 0.000

MgSO4 6.853e-006 6.861e-006 -5.164 -5.164 0.000

NaSO4- 3.720e-009 3.454e-009 -8.430 -8.462 -0.032

KSO4- 1.807e-009 1.678e-009 -8.743 -8.775 -0.032

HSO4- 3.525e-011 3.273e-011 -10.453 -10.485 -0.032

CaHSO4+ 3.218e-013 2.988e-013 -12.492 -12.525 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.73 -7.64 -8.36 CaCO3

Calcite 0.87 -7.64 -8.50 CaCO3

CO2(g) -3.11 -4.63 -1.51 CO2

Dolomite 1.59 -15.59 -17.18 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.74 -27.91 -3.17 H2

H2O(g) -1.41 -0.00 1.41 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.73 -3.65 -2.92 O2

Initial solution 39. 29/8/2012 21:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.682e-004 4.682e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.360

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 321

Density (g/cm3) = 0.99624

Activity of water = 1.000

Ionic strength = 4.724e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.929e-003

Total CO2 (mol/kg) = 2.929e-003

Temperature (deg C) = 28.700

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.75

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551591e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9497 0.7157

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.253e-006 3.018e-006 -5.488 -5.520 -0.033

H+ 4.670e-009 4.365e-009 -8.331 -8.360 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.929e-003

HCO3- 2.773e-003 2.579e-003 -2.557 -2.589 -0.031

CaCO3 4.105e-005 4.110e-005 -4.387 -4.386 0.000

CO3-2 3.973e-005 2.975e-005 -4.401 -4.527 -0.126

CaHCO3+ 2.832e-005 2.634e-005 -4.548 -4.579 -0.031

CO2 2.425e-005 2.428e-005 -4.615 -4.615 0.000

MgHCO3+ 1.213e-005 1.126e-005 -4.916 -4.949 -0.032

MgCO3 1.100e-005 1.101e-005 -4.959 -4.958 0.000

NaHCO3 1.344e-008 1.345e-008 -7.872 -7.871 0.000

NaCO3- 6.654e-009 6.178e-009 -8.177 -8.209 -0.032

Ca 1.096e-003

Ca+2 1.015e-003 7.599e-004 -2.993 -3.119 -0.126

CaCO3 4.105e-005 4.110e-005 -4.387 -4.386 0.000

CaHCO3+ 2.832e-005 2.634e-005 -4.548 -4.579 -0.031

CaSO4 1.137e-005 1.138e-005 -4.944 -4.944 0.000

CaOH+ 3.112e-008 2.889e-008 -7.507 -7.539 -0.032

CaHSO4+ 3.289e-013 3.053e-013 -12.483 -12.515 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 2.599e-028

H2 1.299e-028 1.301e-028 -27.886 -27.886 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.805e-009 1.675e-009 -8.744 -8.776 -0.032

KOH 2.446e-012 2.449e-012 -11.611 -11.611 0.000

Mg 5.184e-004

Mg+2 4.880e-004 3.664e-004 -3.312 -3.436 -0.124

MgHCO3+ 1.213e-005 1.126e-005 -4.916 -4.949 -0.032

MgCO3 1.100e-005 1.101e-005 -4.959 -4.958 0.000

MgSO4 6.840e-006 6.848e-006 -5.165 -5.164 0.000

MgOH+ 4.566e-007 4.239e-007 -6.340 -6.373 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.344e-008 1.345e-008 -7.872 -7.871 0.000

NaCO3- 6.654e-009 6.178e-009 -8.177 -8.209 -0.032

NaSO4- 3.718e-009 3.452e-009 -8.430 -8.462 -0.032

NaOH 1.402e-011 1.404e-011 -10.853 -10.853 0.000

O(0) 4.682e-004

O2 2.341e-004 2.344e-004 -3.631 -3.630 0.000

S(6) 1.154e-004

SO4-2 9.715e-005 7.255e-005 -4.013 -4.139 -0.127

CaSO4 1.137e-005 1.138e-005 -4.944 -4.944 0.000

MgSO4 6.840e-006 6.848e-006 -5.165 -5.164 0.000

NaSO4- 3.718e-009 3.452e-009 -8.430 -8.462 -0.032

KSO4- 1.805e-009 1.675e-009 -8.744 -8.776 -0.032

HSO4- 3.600e-011 3.342e-011 -10.444 -10.476 -0.032

CaHSO4+ 3.289e-013 3.053e-013 -12.483 -12.515 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.71 -7.65 -8.36 CaCO3

Calcite 0.86 -7.65 -8.50 CaCO3

CO2(g) -3.10 -4.61 -1.51 CO2

Dolomite 1.57 -15.61 -17.17 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.72 -27.89 -3.17 H2

H2O(g) -1.42 -0.00 1.42 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.71 -3.63 -2.92 O2

Initial solution 40. 29/8/2012 21:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.482e-004 4.482e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.350

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 321

Density (g/cm3) = 0.99627

Activity of water = 1.000

Ionic strength = 4.727e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.932e-003

Total CO2 (mol/kg) = 2.932e-003

Temperature (deg C) = 28.600

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.75

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551590e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9631 0.7162

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.156e-006 2.928e-006 -5.501 -5.534 -0.033

H+ 4.778e-009 4.467e-009 -8.321 -8.350 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.932e-003

HCO3- 2.777e-003 2.583e-003 -2.556 -2.588 -0.031

CaCO3 4.005e-005 4.010e-005 -4.397 -4.397 0.000

CO3-2 3.881e-005 2.907e-005 -4.411 -4.537 -0.126

CaHCO3+ 2.835e-005 2.638e-005 -4.547 -4.579 -0.031

CO2 2.488e-005 2.491e-005 -4.604 -4.604 0.000

MgHCO3+ 1.214e-005 1.128e-005 -4.916 -4.948 -0.032

MgCO3 1.074e-005 1.075e-005 -4.969 -4.969 0.000

NaHCO3 1.346e-008 1.347e-008 -7.871 -7.871 0.000

NaCO3- 6.469e-009 6.006e-009 -8.189 -8.221 -0.032

Ca 1.096e-003

Ca+2 1.016e-003 7.606e-004 -2.993 -3.119 -0.126

CaCO3 4.005e-005 4.010e-005 -4.397 -4.397 0.000

CaHCO3+ 2.835e-005 2.638e-005 -4.547 -4.579 -0.031

CaSO4 1.137e-005 1.138e-005 -4.944 -4.944 0.000

CaOH+ 3.044e-008 2.826e-008 -7.517 -7.549 -0.032

CaHSO4+ 3.361e-013 3.121e-013 -12.474 -12.506 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 2.724e-028

H2 1.362e-028 1.363e-028 -27.866 -27.865 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.802e-009 1.673e-009 -8.744 -8.777 -0.032

KOH 2.391e-012 2.393e-012 -11.621 -11.621 0.000

Mg 5.184e-004

Mg+2 4.882e-004 3.666e-004 -3.311 -3.436 -0.124

MgHCO3+ 1.214e-005 1.128e-005 -4.916 -4.948 -0.032

MgCO3 1.074e-005 1.075e-005 -4.969 -4.969 0.000

MgSO4 6.827e-006 6.835e-006 -5.166 -5.165 0.000

MgOH+ 4.425e-007 4.109e-007 -6.354 -6.386 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.346e-008 1.347e-008 -7.871 -7.871 0.000

NaCO3- 6.469e-009 6.006e-009 -8.189 -8.221 -0.032

NaSO4- 3.716e-009 3.450e-009 -8.430 -8.462 -0.032

NaOH 1.370e-011 1.372e-011 -10.863 -10.863 0.000

O(0) 4.482e-004

O2 2.241e-004 2.244e-004 -3.650 -3.649 0.000

S(6) 1.154e-004

SO4-2 9.717e-005 7.256e-005 -4.012 -4.139 -0.127

CaSO4 1.137e-005 1.138e-005 -4.944 -4.944 0.000

MgSO4 6.827e-006 6.835e-006 -5.166 -5.165 0.000

NaSO4- 3.716e-009 3.450e-009 -8.430 -8.462 -0.032

KSO4- 1.802e-009 1.673e-009 -8.744 -8.777 -0.032

HSO4- 3.676e-011 3.413e-011 -10.435 -10.467 -0.032

CaHSO4+ 3.361e-013 3.121e-013 -12.474 -12.506 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.70 -7.66 -8.36 CaCO3

Calcite 0.85 -7.66 -8.50 CaCO3

CO2(g) -3.09 -4.60 -1.51 CO2

Dolomite 1.54 -15.63 -17.17 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.70 -27.87 -3.17 H2

H2O(g) -1.42 -0.00 1.42 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.73 -3.65 -2.92 O2

Initial solution 41. 29/8/2012 21:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.990e-003 2.990e-003

Ca 1.092e-003 1.092e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.795e-004 4.795e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.340

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 319

Density (g/cm3) = 0.99630

Activity of water = 1.000

Ionic strength = 4.718e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.925e-003

Total CO2 (mol/kg) = 2.925e-003

Temperature (deg C) = 28.500

Electrical balance (eq) = -4.336e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.70

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551591e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9885 0.7175

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.062e-006 2.840e-006 -5.514 -5.547 -0.033

H+ 4.889e-009 4.571e-009 -8.311 -8.340 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.925e-003

HCO3- 2.772e-003 2.579e-003 -2.557 -2.589 -0.031

CaCO3 3.884e-005 3.888e-005 -4.411 -4.410 0.000

CO3-2 3.779e-005 2.830e-005 -4.423 -4.548 -0.125

CaHCO3+ 2.821e-005 2.624e-005 -4.550 -4.581 -0.031

CO2 2.545e-005 2.548e-005 -4.594 -4.594 0.000

MgHCO3+ 1.213e-005 1.126e-005 -4.916 -4.948 -0.032

MgCO3 1.045e-005 1.046e-005 -4.981 -4.980 0.000

NaHCO3 1.344e-008 1.345e-008 -7.872 -7.871 0.000

NaCO3- 6.269e-009 5.821e-009 -8.203 -8.235 -0.032

Ca 1.092e-003

Ca+2 1.014e-003 7.591e-004 -2.994 -3.120 -0.126

CaCO3 3.884e-005 3.888e-005 -4.411 -4.410 0.000

CaHCO3+ 2.821e-005 2.624e-005 -4.550 -4.581 -0.031

CaSO4 1.135e-005 1.136e-005 -4.945 -4.945 0.000

CaOH+ 2.968e-008 2.756e-008 -7.528 -7.560 -0.032

CaHSO4+ 3.427e-013 3.182e-013 -12.465 -12.497 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 2.855e-028

H2 1.427e-028 1.429e-028 -27.845 -27.845 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.800e-009 1.671e-009 -8.745 -8.777 -0.032

KOH 2.337e-012 2.339e-012 -11.631 -11.631 0.000

Mg 5.184e-004

Mg+2 4.886e-004 3.670e-004 -3.311 -3.435 -0.124

MgHCO3+ 1.213e-005 1.126e-005 -4.916 -4.948 -0.032

MgCO3 1.045e-005 1.046e-005 -4.981 -4.980 0.000

MgSO4 6.821e-006 6.828e-006 -5.166 -5.166 0.000

MgOH+ 4.290e-007 3.984e-007 -6.368 -6.400 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.344e-008 1.345e-008 -7.872 -7.871 0.000

NaCO3- 6.269e-009 5.821e-009 -8.203 -8.235 -0.032

NaSO4- 3.716e-009 3.450e-009 -8.430 -8.462 -0.032

NaOH 1.339e-011 1.341e-011 -10.873 -10.873 0.000

O(0) 4.795e-004

O2 2.397e-004 2.400e-004 -3.620 -3.620 0.000

S(6) 1.154e-004

SO4-2 9.720e-005 7.261e-005 -4.012 -4.139 -0.127

CaSO4 1.135e-005 1.136e-005 -4.945 -4.945 0.000

MgSO4 6.821e-006 6.828e-006 -5.166 -5.166 0.000

NaSO4- 3.716e-009 3.450e-009 -8.430 -8.462 -0.032

KSO4- 1.800e-009 1.671e-009 -8.745 -8.777 -0.032

HSO4- 3.755e-011 3.486e-011 -10.425 -10.458 -0.032

CaHSO4+ 3.427e-013 3.182e-013 -12.465 -12.497 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.69 -7.67 -8.36 CaCO3

Calcite 0.83 -7.67 -8.50 CaCO3

CO2(g) -3.09 -4.59 -1.51 CO2

Dolomite 1.52 -15.65 -17.17 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.68 -27.84 -3.16 H2

H2O(g) -1.42 -0.00 1.42 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.70 -3.62 -2.92 O2

Initial solution 42. 29/8/2012 22:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.345e-004 4.345e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.340

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 320

Density (g/cm3) = 0.99630

Activity of water = 1.000

Ionic strength = 4.730e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.935e-003

Total CO2 (mol/kg) = 2.935e-003

Temperature (deg C) = 28.500

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.75

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551590e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9778 0.7169

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.062e-006 2.840e-006 -5.514 -5.547 -0.033

H+ 4.890e-009 4.571e-009 -8.311 -8.340 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.935e-003

HCO3- 2.781e-003 2.587e-003 -2.556 -2.587 -0.031

CaCO3 3.908e-005 3.912e-005 -4.408 -4.408 0.000

CO3-2 3.792e-005 2.840e-005 -4.421 -4.547 -0.126

CaHCO3+ 2.839e-005 2.641e-005 -4.547 -4.578 -0.031

CO2 2.553e-005 2.556e-005 -4.593 -4.592 0.000

MgHCO3+ 1.216e-005 1.129e-005 -4.915 -4.947 -0.032

MgCO3 1.048e-005 1.049e-005 -4.980 -4.979 0.000

NaHCO3 1.348e-008 1.349e-008 -7.870 -7.870 0.000

NaCO3- 6.289e-009 5.839e-009 -8.201 -8.234 -0.032

Ca 1.096e-003

Ca+2 1.017e-003 7.613e-004 -2.993 -3.118 -0.126

CaCO3 3.908e-005 3.912e-005 -4.408 -4.408 0.000

CaHCO3+ 2.839e-005 2.641e-005 -4.547 -4.578 -0.031

CaSO4 1.137e-005 1.139e-005 -4.944 -4.944 0.000

CaOH+ 2.977e-008 2.764e-008 -7.526 -7.558 -0.032

CaHSO4+ 3.435e-013 3.189e-013 -12.464 -12.496 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 2.855e-028

H2 1.427e-028 1.429e-028 -27.845 -27.845 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.799e-009 1.670e-009 -8.745 -8.777 -0.032

KOH 2.336e-012 2.339e-012 -11.631 -11.631 0.000

Mg 5.184e-004

Mg+2 4.885e-004 3.668e-004 -3.311 -3.436 -0.124

MgHCO3+ 1.216e-005 1.129e-005 -4.915 -4.947 -0.032

MgCO3 1.048e-005 1.049e-005 -4.980 -4.979 0.000

MgSO4 6.814e-006 6.822e-006 -5.167 -5.166 0.000

MgOH+ 4.289e-007 3.982e-007 -6.368 -6.400 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.348e-008 1.349e-008 -7.870 -7.870 0.000

NaCO3- 6.289e-009 5.839e-009 -8.201 -8.234 -0.032

NaSO4- 3.714e-009 3.448e-009 -8.430 -8.462 -0.032

NaOH 1.339e-011 1.341e-011 -10.873 -10.873 0.000

O(0) 4.345e-004

O2 2.172e-004 2.175e-004 -3.663 -3.663 0.000

S(6) 1.154e-004

SO4-2 9.718e-005 7.257e-005 -4.012 -4.139 -0.127

CaSO4 1.137e-005 1.139e-005 -4.944 -4.944 0.000

MgSO4 6.814e-006 6.822e-006 -5.167 -5.166 0.000

NaSO4- 3.714e-009 3.448e-009 -8.430 -8.462 -0.032

KSO4- 1.799e-009 1.670e-009 -8.745 -8.777 -0.032

HSO4- 3.753e-011 3.485e-011 -10.426 -10.458 -0.032

CaHSO4+ 3.435e-013 3.189e-013 -12.464 -12.496 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.69 -7.67 -8.36 CaCO3

Calcite 0.84 -7.67 -8.50 CaCO3

CO2(g) -3.08 -4.59 -1.51 CO2

Dolomite 1.52 -15.65 -17.17 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.68 -27.84 -3.16 H2

H2O(g) -1.42 -0.00 1.42 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.75 -3.66 -2.92 O2

Initial solution 43. 29/8/2012 22:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.357e-004 4.357e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.320

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 320

Density (g/cm3) = 0.99633

Activity of water = 1.000

Ionic strength = 4.734e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.940e-003

Total CO2 (mol/kg) = 2.940e-003

Temperature (deg C) = 28.400

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551591e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.0062 0.7183

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.903e-006 2.693e-006 -5.537 -5.570 -0.033

H+ 5.120e-009 4.786e-009 -8.291 -8.320 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.940e-003

HCO3- 2.789e-003 2.595e-003 -2.555 -2.586 -0.031

CaCO3 3.733e-005 3.737e-005 -4.428 -4.427 0.000

CO3-2 3.625e-005 2.714e-005 -4.441 -4.566 -0.126

CaHCO3+ 2.847e-005 2.649e-005 -4.546 -4.577 -0.031

CO2 2.684e-005 2.686e-005 -4.571 -4.571 0.000

MgHCO3+ 1.220e-005 1.133e-005 -4.914 -4.946 -0.032

MgCO3 1.001e-005 1.002e-005 -5.000 -4.999 0.000

NaHCO3 1.352e-008 1.353e-008 -7.869 -7.869 0.000

NaCO3- 5.982e-009 5.554e-009 -8.223 -8.255 -0.032

Ca 1.096e-003

Ca+2 1.019e-003 7.625e-004 -2.992 -3.118 -0.126

CaCO3 3.733e-005 3.737e-005 -4.428 -4.427 0.000

CaHCO3+ 2.847e-005 2.649e-005 -4.546 -4.577 -0.031

CaSO4 1.138e-005 1.139e-005 -4.944 -4.943 0.000

CaOH+ 2.847e-008 2.644e-008 -7.546 -7.578 -0.032

CaHSO4+ 3.595e-013 3.337e-013 -12.444 -12.477 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 3.133e-028

H2 1.567e-028 1.568e-028 -27.805 -27.805 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.796e-009 1.667e-009 -8.746 -8.778 -0.032

KOH 2.231e-012 2.234e-012 -11.651 -11.651 0.000

Mg 5.184e-004

Mg+2 4.890e-004 3.671e-004 -3.311 -3.435 -0.124

MgHCO3+ 1.220e-005 1.133e-005 -4.914 -4.946 -0.032

MgCO3 1.001e-005 1.002e-005 -5.000 -4.999 0.000

MgSO4 6.803e-006 6.810e-006 -5.167 -5.167 0.000

MgOH+ 4.063e-007 3.773e-007 -6.391 -6.423 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.352e-008 1.353e-008 -7.869 -7.869 0.000

NaCO3- 5.982e-009 5.554e-009 -8.223 -8.255 -0.032

NaSO4- 3.712e-009 3.446e-009 -8.430 -8.463 -0.032

NaOH 1.279e-011 1.280e-011 -10.893 -10.893 0.000

O(0) 4.357e-004

O2 2.179e-004 2.181e-004 -3.662 -3.661 0.000

S(6) 1.154e-004

SO4-2 9.718e-005 7.256e-005 -4.012 -4.139 -0.127

CaSO4 1.138e-005 1.139e-005 -4.944 -4.943 0.000

MgSO4 6.803e-006 6.810e-006 -5.167 -5.167 0.000

NaSO4- 3.712e-009 3.446e-009 -8.430 -8.463 -0.032

KSO4- 1.796e-009 1.667e-009 -8.746 -8.778 -0.032

HSO4- 3.921e-011 3.640e-011 -10.407 -10.439 -0.032

CaHSO4+ 3.595e-013 3.337e-013 -12.444 -12.477 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.67 -7.68 -8.36 CaCO3

Calcite 0.82 -7.68 -8.50 CaCO3

CO2(g) -3.06 -4.57 -1.51 CO2

Dolomite 1.48 -15.69 -17.17 CaMg(CO3)2

Gypsum -2.67 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.64 -27.80 -3.16 H2

H2O(g) -1.42 -0.00 1.42 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.75 -3.66 -2.92 O2

Initial solution 44. 29/8/2012 22:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.751e-004 4.751e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.320

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 320

Density (g/cm3) = 0.99633

Activity of water = 1.000

Ionic strength = 4.734e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.940e-003

Total CO2 (mol/kg) = 2.940e-003

Temperature (deg C) = 28.400

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551595e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.0156 0.7189

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.903e-006 2.693e-006 -5.537 -5.570 -0.033

H+ 5.120e-009 4.786e-009 -8.291 -8.320 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.940e-003

HCO3- 2.789e-003 2.595e-003 -2.555 -2.586 -0.031

CaCO3 3.733e-005 3.737e-005 -4.428 -4.427 0.000

CO3-2 3.625e-005 2.714e-005 -4.441 -4.566 -0.126

CaHCO3+ 2.847e-005 2.649e-005 -4.546 -4.577 -0.031

CO2 2.684e-005 2.686e-005 -4.571 -4.571 0.000

MgHCO3+ 1.220e-005 1.133e-005 -4.914 -4.946 -0.032

MgCO3 1.001e-005 1.002e-005 -5.000 -4.999 0.000

NaHCO3 1.352e-008 1.353e-008 -7.869 -7.869 0.000

NaCO3- 5.982e-009 5.554e-009 -8.223 -8.255 -0.032

Ca 1.096e-003

Ca+2 1.019e-003 7.625e-004 -2.992 -3.118 -0.126

CaCO3 3.733e-005 3.737e-005 -4.428 -4.427 0.000

CaHCO3+ 2.847e-005 2.649e-005 -4.546 -4.577 -0.031

CaSO4 1.138e-005 1.139e-005 -4.944 -4.943 0.000

CaOH+ 2.847e-008 2.644e-008 -7.546 -7.578 -0.032

CaHSO4+ 3.595e-013 3.337e-013 -12.444 -12.477 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 3.133e-028

H2 1.567e-028 1.568e-028 -27.805 -27.805 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.796e-009 1.667e-009 -8.746 -8.778 -0.032

KOH 2.231e-012 2.234e-012 -11.651 -11.651 0.000

Mg 5.184e-004

Mg+2 4.890e-004 3.671e-004 -3.311 -3.435 -0.124

MgHCO3+ 1.220e-005 1.133e-005 -4.914 -4.946 -0.032

MgCO3 1.001e-005 1.002e-005 -5.000 -4.999 0.000

MgSO4 6.803e-006 6.810e-006 -5.167 -5.167 0.000

MgOH+ 4.063e-007 3.773e-007 -6.391 -6.423 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.352e-008 1.353e-008 -7.869 -7.869 0.000

NaCO3- 5.982e-009 5.554e-009 -8.223 -8.255 -0.032

NaSO4- 3.712e-009 3.446e-009 -8.430 -8.463 -0.032

NaOH 1.279e-011 1.280e-011 -10.893 -10.893 0.000

O(0) 4.751e-004

O2 2.376e-004 2.378e-004 -3.624 -3.624 0.000

S(6) 1.154e-004

SO4-2 9.718e-005 7.256e-005 -4.012 -4.139 -0.127

CaSO4 1.138e-005 1.139e-005 -4.944 -4.943 0.000

MgSO4 6.803e-006 6.810e-006 -5.167 -5.167 0.000

NaSO4- 3.712e-009 3.446e-009 -8.430 -8.463 -0.032

KSO4- 1.796e-009 1.667e-009 -8.746 -8.778 -0.032

HSO4- 3.921e-011 3.640e-011 -10.407 -10.439 -0.032

CaHSO4+ 3.595e-013 3.337e-013 -12.444 -12.477 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.67 -7.68 -8.36 CaCO3

Calcite 0.82 -7.68 -8.50 CaCO3

CO2(g) -3.06 -4.57 -1.51 CO2

Dolomite 1.48 -15.69 -17.17 CaMg(CO3)2

Gypsum -2.67 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.64 -27.80 -3.16 H2

H2O(g) -1.42 -0.00 1.42 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.71 -3.62 -2.92 O2

Initial solution 45. 29/8/2012 22:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.526e-004 4.526e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.320

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 320

Density (g/cm3) = 0.99636

Activity of water = 1.000

Ionic strength = 4.747e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.951e-003

Total CO2 (mol/kg) = 2.951e-003

Temperature (deg C) = 28.300

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.79

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551596e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.0184 0.7188

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.882e-006 2.673e-006 -5.540 -5.573 -0.033

H+ 5.121e-009 4.786e-009 -8.291 -8.320 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.951e-003

HCO3- 2.799e-003 2.603e-003 -2.553 -2.584 -0.031

CaCO3 3.742e-005 3.746e-005 -4.427 -4.426 0.000

CO3-2 3.632e-005 2.719e-005 -4.440 -4.566 -0.126

CaHCO3+ 2.862e-005 2.663e-005 -4.543 -4.575 -0.031

CO2 2.696e-005 2.699e-005 -4.569 -4.569 0.000

MgHCO3+ 1.224e-005 1.136e-005 -4.912 -4.945 -0.032

MgCO3 1.001e-005 1.002e-005 -5.000 -4.999 0.000

NaHCO3 1.356e-008 1.358e-008 -7.868 -7.867 0.000

NaCO3- 5.963e-009 5.535e-009 -8.225 -8.257 -0.032

Ca 1.100e-003

Ca+2 1.022e-003 7.649e-004 -2.990 -3.116 -0.126

CaCO3 3.742e-005 3.746e-005 -4.427 -4.426 0.000

CaHCO3+ 2.862e-005 2.663e-005 -4.543 -4.575 -0.031

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

CaOH+ 2.857e-008 2.652e-008 -7.544 -7.576 -0.032

CaHSO4+ 3.597e-013 3.339e-013 -12.444 -12.476 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 3.136e-028

H2 1.568e-028 1.570e-028 -27.805 -27.804 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.792e-009 1.664e-009 -8.747 -8.779 -0.032

KOH 2.231e-012 2.233e-012 -11.652 -11.651 0.000

Mg 5.184e-004

Mg+2 4.890e-004 3.670e-004 -3.311 -3.435 -0.125

MgHCO3+ 1.224e-005 1.136e-005 -4.912 -4.945 -0.032

MgCO3 1.001e-005 1.002e-005 -5.000 -4.999 0.000

MgSO4 6.782e-006 6.789e-006 -5.169 -5.168 0.000

MgOH+ 4.027e-007 3.738e-007 -6.395 -6.427 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.356e-008 1.358e-008 -7.868 -7.867 0.000

NaCO3- 5.963e-009 5.535e-009 -8.225 -8.257 -0.032

NaSO4- 3.708e-009 3.443e-009 -8.431 -8.463 -0.032

NaOH 1.279e-011 1.280e-011 -10.893 -10.893 0.000

O(0) 4.526e-004

O2 2.263e-004 2.266e-004 -3.645 -3.645 0.000

S(6) 1.154e-004

SO4-2 9.718e-005 7.254e-005 -4.012 -4.139 -0.127

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

MgSO4 6.782e-006 6.789e-006 -5.169 -5.168 0.000

NaSO4- 3.708e-009 3.443e-009 -8.431 -8.463 -0.032

KSO4- 1.792e-009 1.664e-009 -8.747 -8.779 -0.032

HSO4- 3.912e-011 3.631e-011 -10.408 -10.440 -0.032

CaHSO4+ 3.597e-013 3.339e-013 -12.444 -12.476 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.68 -7.68 -8.36 CaCO3

Calcite 0.82 -7.68 -8.50 CaCO3

CO2(g) -3.06 -4.57 -1.51 CO2

Dolomite 1.48 -15.68 -17.17 CaMg(CO3)2

Gypsum -2.67 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.64 -27.80 -3.16 H2

H2O(g) -1.43 -0.00 1.43 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.73 -3.64 -2.92 O2

Initial solution 46. 29/8/2012 23:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.445e-004 4.445e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.290

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 320

Density (g/cm3) = 0.99639

Activity of water = 1.000

Ionic strength = 4.753e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.958e-003

Total CO2 (mol/kg) = 2.958e-003

Temperature (deg C) = 28.200

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.79

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551597e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.0546 0.7208

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.670e-006 2.476e-006 -5.573 -5.606 -0.033

H+ 5.487e-009 5.129e-009 -8.261 -8.290 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.958e-003

HCO3- 2.810e-003 2.614e-003 -2.551 -2.583 -0.031

CaCO3 3.499e-005 3.503e-005 -4.456 -4.456 0.000

CO3-2 3.397e-005 2.542e-005 -4.469 -4.595 -0.126

CO2 2.903e-005 2.906e-005 -4.537 -4.537 0.000

CaHCO3+ 2.876e-005 2.675e-005 -4.541 -4.573 -0.031

MgHCO3+ 1.229e-005 1.141e-005 -4.910 -4.943 -0.032

MgCO3 9.354e-006 9.364e-006 -5.029 -5.029 0.000

NaHCO3 1.362e-008 1.363e-008 -7.866 -7.865 0.000

NaCO3- 5.549e-009 5.151e-009 -8.256 -8.288 -0.032

Ca 1.100e-003

Ca+2 1.025e-003 7.665e-004 -2.989 -3.115 -0.126

CaCO3 3.499e-005 3.503e-005 -4.456 -4.456 0.000

CaHCO3+ 2.876e-005 2.675e-005 -4.541 -4.573 -0.031

CaSO4 1.141e-005 1.143e-005 -4.943 -4.942 0.000

CaOH+ 2.672e-008 2.480e-008 -7.573 -7.606 -0.032

CaHSO4+ 3.853e-013 3.577e-013 -12.414 -12.446 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 3.605e-028

H2 1.802e-028 1.804e-028 -27.744 -27.744 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.789e-009 1.661e-009 -8.747 -8.780 -0.032

KOH 2.082e-012 2.084e-012 -11.682 -11.681 0.000

Mg 5.184e-004

Mg+2 4.896e-004 3.675e-004 -3.310 -3.435 -0.125

MgHCO3+ 1.229e-005 1.141e-005 -4.910 -4.943 -0.032

MgCO3 9.354e-006 9.364e-006 -5.029 -5.029 0.000

MgSO4 6.772e-006 6.779e-006 -5.169 -5.169 0.000

MgOH+ 3.730e-007 3.462e-007 -6.428 -6.461 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.362e-008 1.363e-008 -7.866 -7.865 0.000

NaCO3- 5.549e-009 5.151e-009 -8.256 -8.288 -0.032

NaSO4- 3.705e-009 3.440e-009 -8.431 -8.463 -0.032

NaOH 1.193e-011 1.195e-011 -10.923 -10.923 0.000

O(0) 4.445e-004

O2 2.222e-004 2.225e-004 -3.653 -3.653 0.000

S(6) 1.154e-004

SO4-2 9.718e-005 7.253e-005 -4.012 -4.139 -0.127

CaSO4 1.141e-005 1.143e-005 -4.943 -4.942 0.000

MgSO4 6.772e-006 6.779e-006 -5.169 -5.169 0.000

NaSO4- 3.705e-009 3.440e-009 -8.431 -8.463 -0.032

KSO4- 1.789e-009 1.661e-009 -8.747 -8.780 -0.032

HSO4- 4.181e-011 3.882e-011 -10.379 -10.411 -0.032

CaHSO4+ 3.853e-013 3.577e-013 -12.414 -12.446 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.38 CaSO4

Aragonite 0.65 -7.71 -8.36 CaCO3

Calcite 0.79 -7.71 -8.50 CaCO3

CO2(g) -3.03 -4.54 -1.50 CO2

Dolomite 1.42 -15.74 -17.16 CaMg(CO3)2

Gypsum -2.67 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.58 -27.74 -3.16 H2

H2O(g) -1.43 -0.00 1.43 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.74 -3.65 -2.91 O2

Initial solution 47. 29/8/2012 23:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.551e-004 4.551e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.310

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 319

Density (g/cm3) = 0.99639

Activity of water = 1.000

Ionic strength = 4.738e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.943e-003

Total CO2 (mol/kg) = 2.943e-003

Temperature (deg C) = 28.200

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551594e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.0371 0.7197

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.796e-006 2.593e-006 -5.554 -5.586 -0.033

H+ 5.239e-009 4.898e-009 -8.281 -8.310 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.943e-003

HCO3- 2.794e-003 2.599e-003 -2.554 -2.585 -0.031

CaCO3 3.628e-005 3.632e-005 -4.440 -4.440 0.000

CO3-2 3.535e-005 2.647e-005 -4.452 -4.577 -0.126

CaHCO3+ 2.847e-005 2.649e-005 -4.546 -4.577 -0.031

CO2 2.756e-005 2.759e-005 -4.560 -4.559 0.000

MgHCO3+ 1.222e-005 1.134e-005 -4.913 -4.945 -0.032

MgCO3 9.737e-006 9.747e-006 -5.012 -5.011 0.000

NaHCO3 1.354e-008 1.356e-008 -7.868 -7.868 0.000

NaCO3- 5.777e-009 5.364e-009 -8.238 -8.271 -0.032

Ca 1.096e-003

Ca+2 1.020e-003 7.633e-004 -2.991 -3.117 -0.126

CaCO3 3.628e-005 3.632e-005 -4.440 -4.440 0.000

CaHCO3+ 2.847e-005 2.649e-005 -4.546 -4.577 -0.031

CaSO4 1.137e-005 1.139e-005 -4.944 -4.944 0.000

CaOH+ 2.786e-008 2.586e-008 -7.555 -7.587 -0.032

CaHSO4+ 3.667e-013 3.404e-013 -12.436 -12.468 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 3.287e-028

H2 1.644e-028 1.646e-028 -27.784 -27.784 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.790e-009 1.662e-009 -8.747 -8.779 -0.032

KOH 2.180e-012 2.183e-012 -11.661 -11.661 0.000

Mg 5.184e-004

Mg+2 4.893e-004 3.674e-004 -3.310 -3.435 -0.124

MgHCO3+ 1.222e-005 1.134e-005 -4.913 -4.945 -0.032

MgCO3 9.737e-006 9.747e-006 -5.012 -5.011 0.000

MgSO4 6.775e-006 6.783e-006 -5.169 -5.169 0.000

MgOH+ 3.904e-007 3.624e-007 -6.409 -6.441 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.354e-008 1.356e-008 -7.868 -7.868 0.000

NaCO3- 5.777e-009 5.364e-009 -8.238 -8.271 -0.032

NaSO4- 3.708e-009 3.443e-009 -8.431 -8.463 -0.032

NaOH 1.250e-011 1.251e-011 -10.903 -10.903 0.000

O(0) 4.551e-004

O2 2.276e-004 2.278e-004 -3.643 -3.642 0.000

S(6) 1.154e-004

SO4-2 9.721e-005 7.259e-005 -4.012 -4.139 -0.127

CaSO4 1.137e-005 1.139e-005 -4.944 -4.944 0.000

MgSO4 6.775e-006 6.783e-006 -5.169 -5.169 0.000

NaSO4- 3.708e-009 3.443e-009 -8.431 -8.463 -0.032

KSO4- 1.790e-009 1.662e-009 -8.747 -8.779 -0.032

HSO4- 3.996e-011 3.710e-011 -10.398 -10.431 -0.032

CaHSO4+ 3.667e-013 3.404e-013 -12.436 -12.468 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.66 -7.69 -8.36 CaCO3

Calcite 0.80 -7.69 -8.50 CaCO3

CO2(g) -3.05 -4.56 -1.50 CO2

Dolomite 1.46 -15.71 -17.16 CaMg(CO3)2

Gypsum -2.67 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.62 -27.78 -3.16 H2

H2O(g) -1.43 -0.00 1.43 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.73 -3.64 -2.91 O2

Initial solution 48. 29/8/2012 23:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.751e-004 4.751e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.290

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 318

Density (g/cm3) = 0.99642

Activity of water = 1.000

Ionic strength = 4.742e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.949e-003

Total CO2 (mol/kg) = 2.949e-003

Temperature (deg C) = 28.100

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551597e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.0699 0.7214

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.650e-006 2.458e-006 -5.577 -5.609 -0.033

H+ 5.486e-009 5.129e-009 -8.261 -8.290 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.949e-003

HCO3- 2.801e-003 2.606e-003 -2.553 -2.584 -0.031

CaCO3 3.465e-005 3.469e-005 -4.460 -4.460 0.000

CO3-2 3.379e-005 2.530e-005 -4.471 -4.597 -0.126

CO2 2.897e-005 2.900e-005 -4.538 -4.538 0.000

CaHCO3+ 2.855e-005 2.656e-005 -4.544 -4.576 -0.031

MgHCO3+ 1.225e-005 1.138e-005 -4.912 -4.944 -0.032

MgCO3 9.299e-006 9.309e-006 -5.032 -5.031 0.000

NaHCO3 1.358e-008 1.359e-008 -7.867 -7.867 0.000

NaCO3- 5.494e-009 5.101e-009 -8.260 -8.292 -0.032

Ca 1.096e-003

Ca+2 1.021e-003 7.644e-004 -2.991 -3.117 -0.126

CaCO3 3.465e-005 3.469e-005 -4.460 -4.460 0.000

CaHCO3+ 2.855e-005 2.656e-005 -4.544 -4.576 -0.031

CaSO4 1.138e-005 1.139e-005 -4.944 -4.943 0.000

CaOH+ 2.664e-008 2.473e-008 -7.574 -7.607 -0.032

CaHSO4+ 3.837e-013 3.562e-013 -12.416 -12.448 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 3.608e-028

H2 1.804e-028 1.806e-028 -27.744 -27.743 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.787e-009 1.659e-009 -8.748 -8.780 -0.032

KOH 2.082e-012 2.084e-012 -11.681 -11.681 0.000

Mg 5.184e-004

Mg+2 4.897e-004 3.677e-004 -3.310 -3.435 -0.124

MgHCO3+ 1.225e-005 1.138e-005 -4.912 -4.944 -0.032

MgCO3 9.299e-006 9.309e-006 -5.032 -5.031 0.000

MgSO4 6.764e-006 6.771e-006 -5.170 -5.169 0.000

MgOH+ 3.698e-007 3.434e-007 -6.432 -6.464 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.358e-008 1.359e-008 -7.867 -7.867 0.000

NaCO3- 5.494e-009 5.101e-009 -8.260 -8.292 -0.032

NaSO4- 3.706e-009 3.441e-009 -8.431 -8.463 -0.032

NaOH 1.194e-011 1.195e-011 -10.923 -10.923 0.000

O(0) 4.751e-004

O2 2.376e-004 2.378e-004 -3.624 -3.624 0.000

S(6) 1.154e-004

SO4-2 9.722e-005 7.259e-005 -4.012 -4.139 -0.127

CaSO4 1.138e-005 1.139e-005 -4.944 -4.943 0.000

MgSO4 6.764e-006 6.771e-006 -5.170 -5.169 0.000

NaSO4- 3.706e-009 3.441e-009 -8.431 -8.463 -0.032

KSO4- 1.787e-009 1.659e-009 -8.748 -8.780 -0.032

HSO4- 4.175e-011 3.876e-011 -10.379 -10.412 -0.032

CaHSO4+ 3.837e-013 3.562e-013 -12.416 -12.448 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.64 -7.71 -8.36 CaCO3

Calcite 0.78 -7.71 -8.50 CaCO3

CO2(g) -3.03 -4.54 -1.50 CO2

Dolomite 1.42 -15.75 -17.16 CaMg(CO3)2

Gypsum -2.67 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.58 -27.74 -3.16 H2

H2O(g) -1.43 -0.00 1.43 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.71 -3.62 -2.91 O2

Initial solution 49. 29/8/2012 23:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.476e-004 4.476e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.300

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 319

Density (g/cm3) = 0.99642

Activity of water = 1.000

Ionic strength = 4.752e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.956e-003

Total CO2 (mol/kg) = 2.956e-003

Temperature (deg C) = 28.100

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.79

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551597e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.0534 0.7204

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.712e-006 2.516e-006 -5.567 -5.599 -0.033

H+ 5.362e-009 5.012e-009 -8.271 -8.300 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.956e-003

HCO3- 2.807e-003 2.611e-003 -2.552 -2.583 -0.031

CaCO3 3.561e-005 3.565e-005 -4.448 -4.448 0.000

CO3-2 3.466e-005 2.594e-005 -4.460 -4.586 -0.126

CaHCO3+ 2.868e-005 2.668e-005 -4.542 -4.574 -0.031

CO2 2.837e-005 2.840e-005 -4.547 -4.547 0.000

MgHCO3+ 1.227e-005 1.139e-005 -4.911 -4.943 -0.032

MgCO3 9.528e-006 9.538e-006 -5.021 -5.021 0.000

NaHCO3 1.360e-008 1.362e-008 -7.866 -7.866 0.000

NaCO3- 5.634e-009 5.230e-009 -8.249 -8.281 -0.032

Ca 1.100e-003

Ca+2 1.024e-003 7.662e-004 -2.990 -3.116 -0.126

CaCO3 3.561e-005 3.565e-005 -4.448 -4.448 0.000

CaHCO3+ 2.868e-005 2.668e-005 -4.542 -4.574 -0.031

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

CaOH+ 2.733e-008 2.537e-008 -7.563 -7.596 -0.032

CaHSO4+ 3.757e-013 3.488e-013 -12.425 -12.457 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 3.446e-028

H2 1.723e-028 1.725e-028 -27.764 -27.763 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.786e-009 1.658e-009 -8.748 -8.780 -0.032

KOH 2.131e-012 2.133e-012 -11.672 -11.671 0.000

Mg 5.184e-004

Mg+2 4.895e-004 3.674e-004 -3.310 -3.435 -0.125

MgHCO3+ 1.227e-005 1.139e-005 -4.911 -4.943 -0.032

MgCO3 9.528e-006 9.538e-006 -5.021 -5.021 0.000

MgSO4 6.756e-006 6.763e-006 -5.170 -5.170 0.000

MgOH+ 3.782e-007 3.511e-007 -6.422 -6.455 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.360e-008 1.362e-008 -7.866 -7.866 0.000

NaCO3- 5.634e-009 5.230e-009 -8.249 -8.281 -0.032

NaSO4- 3.705e-009 3.439e-009 -8.431 -8.464 -0.032

NaOH 1.221e-011 1.223e-011 -10.913 -10.913 0.000

O(0) 4.476e-004

O2 2.238e-004 2.241e-004 -3.650 -3.650 0.000

S(6) 1.154e-004

SO4-2 9.721e-005 7.256e-005 -4.012 -4.139 -0.127

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

MgSO4 6.756e-006 6.763e-006 -5.170 -5.170 0.000

NaSO4- 3.705e-009 3.439e-009 -8.431 -8.464 -0.032

KSO4- 1.786e-009 1.658e-009 -8.748 -8.780 -0.032

HSO4- 4.078e-011 3.786e-011 -10.390 -10.422 -0.032

CaHSO4+ 3.757e-013 3.488e-013 -12.425 -12.457 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.38 CaSO4

Aragonite 0.65 -7.70 -8.36 CaCO3

Calcite 0.80 -7.70 -8.50 CaCO3

CO2(g) -3.04 -4.55 -1.50 CO2

Dolomite 1.44 -15.72 -17.16 CaMg(CO3)2

Gypsum -2.67 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.60 -27.76 -3.16 H2

H2O(g) -1.43 -0.00 1.43 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.74 -3.65 -2.91 O2

Initial solution 50. 30/8/2012 00:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.751e-004 4.751e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.300

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 317

Density (g/cm3) = 0.99645

Activity of water = 1.000

Ionic strength = 4.741e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.946e-003

Total CO2 (mol/kg) = 2.946e-003

Temperature (deg C) = 28.000

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551597e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.0680 0.7211

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.692e-006 2.497e-006 -5.570 -5.603 -0.033

H+ 5.361e-009 5.012e-009 -8.271 -8.300 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.946e-003

HCO3- 2.798e-003 2.603e-003 -2.553 -2.585 -0.031

CaCO3 3.526e-005 3.530e-005 -4.453 -4.452 0.000

CO3-2 3.447e-005 2.581e-005 -4.463 -4.588 -0.126

CaHCO3+ 2.847e-005 2.649e-005 -4.546 -4.577 -0.031

CO2 2.831e-005 2.834e-005 -4.548 -4.548 0.000

MgHCO3+ 1.223e-005 1.136e-005 -4.913 -4.945 -0.032

MgCO3 9.472e-006 9.482e-006 -5.024 -5.023 0.000

NaHCO3 1.356e-008 1.358e-008 -7.868 -7.867 0.000

NaCO3- 5.578e-009 5.179e-009 -8.253 -8.286 -0.032

Ca 1.096e-003

Ca+2 1.021e-003 7.641e-004 -2.991 -3.117 -0.126

CaCO3 3.526e-005 3.530e-005 -4.453 -4.452 0.000

CaHCO3+ 2.847e-005 2.649e-005 -4.546 -4.577 -0.031

CaSO4 1.137e-005 1.138e-005 -4.944 -4.944 0.000

CaOH+ 2.725e-008 2.530e-008 -7.565 -7.597 -0.032

CaHSO4+ 3.741e-013 3.473e-013 -12.427 -12.459 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 3.449e-028

H2 1.725e-028 1.726e-028 -27.763 -27.763 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.785e-009 1.657e-009 -8.748 -8.781 -0.032

KOH 2.131e-012 2.133e-012 -11.671 -11.671 0.000

Mg 5.184e-004

Mg+2 4.896e-004 3.676e-004 -3.310 -3.435 -0.124

MgHCO3+ 1.223e-005 1.136e-005 -4.913 -4.945 -0.032

MgCO3 9.472e-006 9.482e-006 -5.024 -5.023 0.000

MgSO4 6.748e-006 6.755e-006 -5.171 -5.170 0.000

MgOH+ 3.750e-007 3.482e-007 -6.426 -6.458 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.356e-008 1.358e-008 -7.868 -7.867 0.000

NaCO3- 5.578e-009 5.179e-009 -8.253 -8.286 -0.032

NaSO4- 3.705e-009 3.440e-009 -8.431 -8.463 -0.032

NaOH 1.221e-011 1.223e-011 -10.913 -10.913 0.000

O(0) 4.751e-004

O2 2.376e-004 2.378e-004 -3.624 -3.624 0.000

S(6) 1.154e-004

SO4-2 9.725e-005 7.262e-005 -4.012 -4.139 -0.127

CaSO4 1.137e-005 1.138e-005 -4.944 -4.944 0.000

MgSO4 6.748e-006 6.755e-006 -5.171 -5.170 0.000

NaSO4- 3.705e-009 3.440e-009 -8.431 -8.463 -0.032

KSO4- 1.785e-009 1.657e-009 -8.748 -8.781 -0.032

HSO4- 4.072e-011 3.781e-011 -10.390 -10.422 -0.032

CaHSO4+ 3.741e-013 3.473e-013 -12.427 -12.459 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.37 CaSO4

Aragonite 0.65 -7.71 -8.36 CaCO3

Calcite 0.79 -7.71 -8.50 CaCO3

CO2(g) -3.05 -4.55 -1.50 CO2

Dolomite 1.43 -15.73 -17.16 CaMg(CO3)2

Gypsum -2.67 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.60 -27.76 -3.16 H2

H2O(g) -1.43 -0.00 1.43 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.71 -3.62 -2.91 O2

Initial solution 51. 30/8/2012 00:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.939e-004 4.939e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.300

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 317

Density (g/cm3) = 0.99645

Activity of water = 1.000

Ionic strength = 4.741e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.946e-003

Total CO2 (mol/kg) = 2.946e-003

Temperature (deg C) = 28.000

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551599e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.0722 0.7213

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.692e-006 2.497e-006 -5.570 -5.603 -0.033

H+ 5.361e-009 5.012e-009 -8.271 -8.300 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.946e-003

HCO3- 2.798e-003 2.603e-003 -2.553 -2.585 -0.031

CaCO3 3.526e-005 3.530e-005 -4.453 -4.452 0.000

CO3-2 3.447e-005 2.581e-005 -4.463 -4.588 -0.126

CaHCO3+ 2.847e-005 2.649e-005 -4.546 -4.577 -0.031

CO2 2.831e-005 2.834e-005 -4.548 -4.548 0.000

MgHCO3+ 1.223e-005 1.136e-005 -4.913 -4.945 -0.032

MgCO3 9.472e-006 9.482e-006 -5.024 -5.023 0.000

NaHCO3 1.356e-008 1.358e-008 -7.868 -7.867 0.000

NaCO3- 5.578e-009 5.179e-009 -8.253 -8.286 -0.032

Ca 1.096e-003

Ca+2 1.021e-003 7.641e-004 -2.991 -3.117 -0.126

CaCO3 3.526e-005 3.530e-005 -4.453 -4.452 0.000

CaHCO3+ 2.847e-005 2.649e-005 -4.546 -4.577 -0.031

CaSO4 1.137e-005 1.138e-005 -4.944 -4.944 0.000

CaOH+ 2.725e-008 2.530e-008 -7.565 -7.597 -0.032

CaHSO4+ 3.741e-013 3.473e-013 -12.427 -12.459 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 3.449e-028

H2 1.725e-028 1.726e-028 -27.763 -27.763 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.785e-009 1.657e-009 -8.748 -8.781 -0.032

KOH 2.131e-012 2.133e-012 -11.671 -11.671 0.000

Mg 5.184e-004

Mg+2 4.896e-004 3.676e-004 -3.310 -3.435 -0.124

MgHCO3+ 1.223e-005 1.136e-005 -4.913 -4.945 -0.032

MgCO3 9.472e-006 9.482e-006 -5.024 -5.023 0.000

MgSO4 6.748e-006 6.755e-006 -5.171 -5.170 0.000

MgOH+ 3.750e-007 3.482e-007 -6.426 -6.458 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.356e-008 1.358e-008 -7.868 -7.867 0.000

NaCO3- 5.578e-009 5.179e-009 -8.253 -8.286 -0.032

NaSO4- 3.705e-009 3.440e-009 -8.431 -8.463 -0.032

NaOH 1.221e-011 1.223e-011 -10.913 -10.913 0.000

O(0) 4.939e-004

O2 2.469e-004 2.472e-004 -3.607 -3.607 0.000

S(6) 1.154e-004

SO4-2 9.725e-005 7.262e-005 -4.012 -4.139 -0.127

CaSO4 1.137e-005 1.138e-005 -4.944 -4.944 0.000

MgSO4 6.748e-006 6.755e-006 -5.171 -5.170 0.000

NaSO4- 3.705e-009 3.440e-009 -8.431 -8.463 -0.032

KSO4- 1.785e-009 1.657e-009 -8.748 -8.781 -0.032

HSO4- 4.072e-011 3.781e-011 -10.390 -10.422 -0.032

CaHSO4+ 3.741e-013 3.473e-013 -12.427 -12.459 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.37 CaSO4

Aragonite 0.65 -7.71 -8.36 CaCO3

Calcite 0.79 -7.71 -8.50 CaCO3

CO2(g) -3.05 -4.55 -1.50 CO2

Dolomite 1.43 -15.73 -17.16 CaMg(CO3)2

Gypsum -2.67 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.60 -27.76 -3.16 H2

H2O(g) -1.43 -0.00 1.43 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.69 -3.61 -2.91 O2

Initial solution 52. 30/8/2012 00:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.701e-004 4.701e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.290

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 317

Density (g/cm3) = 0.99647

Activity of water = 1.000

Ionic strength = 4.743e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.949e-003

Total CO2 (mol/kg) = 2.949e-003

Temperature (deg C) = 27.900

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551597e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.0850 0.7219

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.612e-006 2.423e-006 -5.583 -5.616 -0.033

H+ 5.486e-009 5.129e-009 -8.261 -8.290 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.949e-003

HCO3- 2.802e-003 2.606e-003 -2.553 -2.584 -0.031

CaCO3 3.439e-005 3.443e-005 -4.464 -4.463 0.000

CO3-2 3.367e-005 2.521e-005 -4.473 -4.598 -0.126

CO2 2.904e-005 2.907e-005 -4.537 -4.537 0.000

CaHCO3+ 2.850e-005 2.651e-005 -4.545 -4.577 -0.031

MgHCO3+ 1.225e-005 1.137e-005 -4.912 -4.944 -0.032

MgCO3 9.242e-006 9.252e-006 -5.034 -5.034 0.000

NaHCO3 1.358e-008 1.360e-008 -7.867 -7.867 0.000

NaCO3- 5.422e-009 5.034e-009 -8.266 -8.298 -0.032

Ca 1.096e-003

Ca+2 1.022e-003 7.647e-004 -2.991 -3.117 -0.126

CaCO3 3.439e-005 3.443e-005 -4.464 -4.463 0.000

CaHCO3+ 2.850e-005 2.651e-005 -4.545 -4.577 -0.031

CaSO4 1.137e-005 1.138e-005 -4.944 -4.944 0.000

CaOH+ 2.665e-008 2.474e-008 -7.574 -7.607 -0.032

CaHSO4+ 3.823e-013 3.549e-013 -12.418 -12.450 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 3.615e-028

H2 1.808e-028 1.810e-028 -27.743 -27.742 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.782e-009 1.654e-009 -8.749 -8.781 -0.032

KOH 2.082e-012 2.084e-012 -11.681 -11.681 0.000

Mg 5.184e-004

Mg+2 4.898e-004 3.678e-004 -3.310 -3.434 -0.124

MgHCO3+ 1.225e-005 1.137e-005 -4.912 -4.944 -0.032

MgCO3 9.242e-006 9.252e-006 -5.034 -5.034 0.000

MgSO4 6.735e-006 6.742e-006 -5.172 -5.171 0.000

MgOH+ 3.634e-007 3.374e-007 -6.440 -6.472 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.358e-008 1.360e-008 -7.867 -7.867 0.000

NaCO3- 5.422e-009 5.034e-009 -8.266 -8.298 -0.032

NaSO4- 3.703e-009 3.438e-009 -8.431 -8.464 -0.032

NaOH 1.194e-011 1.195e-011 -10.923 -10.923 0.000

O(0) 4.701e-004

O2 2.351e-004 2.353e-004 -3.629 -3.628 0.000

S(6) 1.154e-004

SO4-2 9.726e-005 7.262e-005 -4.012 -4.139 -0.127

CaSO4 1.137e-005 1.138e-005 -4.944 -4.944 0.000

MgSO4 6.735e-006 6.742e-006 -5.172 -5.171 0.000

NaSO4- 3.703e-009 3.438e-009 -8.431 -8.464 -0.032

KSO4- 1.782e-009 1.654e-009 -8.749 -8.781 -0.032

HSO4- 4.158e-011 3.861e-011 -10.381 -10.413 -0.032

CaHSO4+ 3.823e-013 3.549e-013 -12.418 -12.450 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.37 CaSO4

Aragonite 0.64 -7.71 -8.36 CaCO3

Calcite 0.78 -7.71 -8.50 CaCO3

CO2(g) -3.04 -4.54 -1.50 CO2

Dolomite 1.41 -15.75 -17.16 CaMg(CO3)2

Gypsum -2.67 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.58 -27.74 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.72 -3.63 -2.91 O2

Initial solution 53. 30/8/2012 00:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.289e-004 5.289e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.280

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 318

Density (g/cm3) = 0.99648

Activity of water = 1.000

Ionic strength = 4.757e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.962e-003

Total CO2 (mol/kg) = 2.962e-003

Temperature (deg C) = 27.900

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.79

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551606e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1078 0.7232

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.553e-006 2.367e-006 -5.593 -5.626 -0.033

H+ 5.615e-009 5.248e-009 -8.251 -8.280 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.962e-003

HCO3- 2.815e-003 2.618e-003 -2.551 -2.582 -0.031

CaCO3 3.388e-005 3.392e-005 -4.470 -4.470 0.000

CO3-2 3.306e-005 2.475e-005 -4.481 -4.606 -0.126

CO2 2.985e-005 2.988e-005 -4.525 -4.525 0.000

CaHCO3+ 2.873e-005 2.672e-005 -4.542 -4.573 -0.031

MgHCO3+ 1.230e-005 1.142e-005 -4.910 -4.942 -0.032

MgCO3 9.070e-006 9.080e-006 -5.042 -5.042 0.000

NaHCO3 1.364e-008 1.365e-008 -7.865 -7.865 0.000

NaCO3- 5.322e-009 4.941e-009 -8.274 -8.306 -0.032

Ca 1.100e-003

Ca+2 1.026e-003 7.674e-004 -2.989 -3.115 -0.126

CaCO3 3.388e-005 3.392e-005 -4.470 -4.470 0.000

CaHCO3+ 2.873e-005 2.672e-005 -4.542 -4.573 -0.031

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

CaOH+ 2.614e-008 2.427e-008 -7.583 -7.615 -0.032

CaHSO4+ 3.924e-013 3.642e-013 -12.406 -12.439 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 3.786e-028

H2 1.893e-028 1.895e-028 -27.723 -27.722 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.781e-009 1.653e-009 -8.749 -8.782 -0.032

KOH 2.035e-012 2.037e-012 -11.692 -11.691 0.000

Mg 5.184e-004

Mg+2 4.899e-004 3.677e-004 -3.310 -3.434 -0.125

MgHCO3+ 1.230e-005 1.142e-005 -4.910 -4.942 -0.032

MgCO3 9.070e-006 9.080e-006 -5.042 -5.042 0.000

MgSO4 6.730e-006 6.737e-006 -5.172 -5.172 0.000

MgOH+ 3.552e-007 3.297e-007 -6.450 -6.482 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.364e-008 1.365e-008 -7.865 -7.865 0.000

NaCO3- 5.322e-009 4.941e-009 -8.274 -8.306 -0.032

NaSO4- 3.701e-009 3.436e-009 -8.432 -8.464 -0.032

NaOH 1.166e-011 1.168e-011 -10.933 -10.933 0.000

O(0) 5.289e-004

O2 2.644e-004 2.647e-004 -3.578 -3.577 0.000

S(6) 1.154e-004

SO4-2 9.723e-005 7.258e-005 -4.012 -4.139 -0.127

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

MgSO4 6.730e-006 6.737e-006 -5.172 -5.172 0.000

NaSO4- 3.701e-009 3.436e-009 -8.432 -8.464 -0.032

KSO4- 1.781e-009 1.653e-009 -8.749 -8.782 -0.032

HSO4- 4.253e-011 3.948e-011 -10.371 -10.404 -0.032

CaHSO4+ 3.924e-013 3.642e-013 -12.406 -12.439 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.63 -7.72 -8.36 CaCO3

Calcite 0.78 -7.72 -8.50 CaCO3

CO2(g) -3.02 -4.52 -1.50 CO2

Dolomite 1.39 -15.76 -17.16 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.56 -27.72 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.66 -3.58 -2.91 O2

Initial solution 54. 30/8/2012 01:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.351e-004 5.351e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.280

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 317

Density (g/cm3) = 0.99650

Activity of water = 1.000

Ionic strength = 4.757e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.962e-003

Total CO2 (mol/kg) = 2.962e-003

Temperature (deg C) = 27.800

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.79

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551607e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1172 0.7235

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.534e-006 2.350e-006 -5.596 -5.629 -0.033

H+ 5.615e-009 5.248e-009 -8.251 -8.280 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.962e-003

HCO3- 2.815e-003 2.618e-003 -2.551 -2.582 -0.031

CaCO3 3.375e-005 3.379e-005 -4.472 -4.471 0.000

CO3-2 3.301e-005 2.471e-005 -4.481 -4.607 -0.126

CO2 2.989e-005 2.992e-005 -4.525 -4.524 0.000

CaHCO3+ 2.870e-005 2.669e-005 -4.542 -4.574 -0.031

MgHCO3+ 1.230e-005 1.142e-005 -4.910 -4.942 -0.032

MgCO3 9.042e-006 9.052e-006 -5.044 -5.043 0.000

NaHCO3 1.364e-008 1.366e-008 -7.865 -7.865 0.000

NaCO3- 5.287e-009 4.908e-009 -8.277 -8.309 -0.032

Ca 1.100e-003

Ca+2 1.026e-003 7.675e-004 -2.989 -3.115 -0.126

CaCO3 3.375e-005 3.379e-005 -4.472 -4.471 0.000

CaHCO3+ 2.870e-005 2.669e-005 -4.542 -4.574 -0.031

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

CaOH+ 2.614e-008 2.427e-008 -7.583 -7.615 -0.032

CaHSO4+ 3.916e-013 3.636e-013 -12.407 -12.439 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 3.789e-028

H2 1.895e-028 1.897e-028 -27.722 -27.722 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.778e-009 1.651e-009 -8.750 -8.782 -0.032

KOH 2.035e-012 2.037e-012 -11.692 -11.691 0.000

Mg 5.184e-004

Mg+2 4.900e-004 3.678e-004 -3.310 -3.434 -0.125

MgHCO3+ 1.230e-005 1.142e-005 -4.910 -4.942 -0.032

MgCO3 9.042e-006 9.052e-006 -5.044 -5.043 0.000

MgSO4 6.715e-006 6.722e-006 -5.173 -5.172 0.000

MgOH+ 3.521e-007 3.269e-007 -6.453 -6.486 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.364e-008 1.366e-008 -7.865 -7.865 0.000

NaCO3- 5.287e-009 4.908e-009 -8.277 -8.309 -0.032

NaSO4- 3.699e-009 3.434e-009 -8.432 -8.464 -0.032

NaOH 1.166e-011 1.168e-011 -10.933 -10.933 0.000

O(0) 5.351e-004

O2 2.676e-004 2.679e-004 -3.573 -3.572 0.000

S(6) 1.154e-004

SO4-2 9.725e-005 7.259e-005 -4.012 -4.139 -0.127

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

MgSO4 6.715e-006 6.722e-006 -5.173 -5.172 0.000

NaSO4- 3.699e-009 3.434e-009 -8.432 -8.464 -0.032

KSO4- 1.778e-009 1.651e-009 -8.750 -8.782 -0.032

HSO4- 4.244e-011 3.940e-011 -10.372 -10.404 -0.032

CaHSO4+ 3.916e-013 3.636e-013 -12.407 -12.439 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.63 -7.72 -8.35 CaCO3

Calcite 0.77 -7.72 -8.50 CaCO3

CO2(g) -3.02 -4.52 -1.50 CO2

Dolomite 1.39 -15.76 -17.15 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.56 -27.72 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.66 -3.57 -2.91 O2

Initial solution 55. 30/8/2012 01:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.501e-004 5.501e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.270

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 317

Density (g/cm3) = 0.99650

Activity of water = 1.000

Ionic strength = 4.759e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.964e-003

Total CO2 (mol/kg) = 2.964e-003

Temperature (deg C) = 27.800

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.79

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551609e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1302 0.7243

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.476e-006 2.297e-006 -5.606 -5.639 -0.033

H+ 5.745e-009 5.370e-009 -8.241 -8.270 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.964e-003

HCO3- 2.818e-003 2.621e-003 -2.550 -2.581 -0.031

CaCO3 3.304e-005 3.308e-005 -4.481 -4.480 0.000

CO3-2 3.229e-005 2.417e-005 -4.491 -4.617 -0.126

CO2 3.062e-005 3.065e-005 -4.514 -4.514 0.000

CaHCO3+ 2.875e-005 2.674e-005 -4.541 -4.573 -0.031

MgHCO3+ 1.232e-005 1.144e-005 -4.909 -4.942 -0.032

MgCO3 8.849e-006 8.859e-006 -5.053 -5.053 0.000

NaHCO3 1.366e-008 1.367e-008 -7.865 -7.864 0.000

NaCO3- 5.172e-009 4.802e-009 -8.286 -8.319 -0.032

Ca 1.100e-003

Ca+2 1.027e-003 7.680e-004 -2.989 -3.115 -0.126

CaCO3 3.304e-005 3.308e-005 -4.481 -4.480 0.000

CaHCO3+ 2.875e-005 2.674e-005 -4.541 -4.573 -0.031

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

CaOH+ 2.556e-008 2.373e-008 -7.592 -7.625 -0.032

CaHSO4+ 4.010e-013 3.722e-013 -12.397 -12.429 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 3.968e-028

H2 1.984e-028 1.986e-028 -27.702 -27.702 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.778e-009 1.650e-009 -8.750 -8.782 -0.032

KOH 1.988e-012 1.990e-012 -11.702 -11.701 0.000

Mg 5.184e-004

Mg+2 4.902e-004 3.679e-004 -3.310 -3.434 -0.125

MgHCO3+ 1.232e-005 1.144e-005 -4.909 -4.942 -0.032

MgCO3 8.849e-006 8.859e-006 -5.053 -5.053 0.000

MgSO4 6.716e-006 6.724e-006 -5.173 -5.172 0.000

MgOH+ 3.442e-007 3.195e-007 -6.463 -6.496 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.366e-008 1.367e-008 -7.865 -7.864 0.000

NaCO3- 5.172e-009 4.802e-009 -8.286 -8.319 -0.032

NaSO4- 3.699e-009 3.434e-009 -8.432 -8.464 -0.032

NaOH 1.140e-011 1.141e-011 -10.943 -10.943 0.000

O(0) 5.501e-004

O2 2.751e-004 2.754e-004 -3.561 -3.560 0.000

S(6) 1.154e-004

SO4-2 9.725e-005 7.258e-005 -4.012 -4.139 -0.127

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

MgSO4 6.716e-006 6.724e-006 -5.173 -5.172 0.000

NaSO4- 3.699e-009 3.434e-009 -8.432 -8.464 -0.032

KSO4- 1.778e-009 1.650e-009 -8.750 -8.782 -0.032

HSO4- 4.343e-011 4.031e-011 -10.362 -10.395 -0.032

CaHSO4+ 4.010e-013 3.722e-013 -12.397 -12.429 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.62 -7.73 -8.35 CaCO3

Calcite 0.76 -7.73 -8.50 CaCO3

CO2(g) -3.01 -4.51 -1.50 CO2

Dolomite 1.37 -15.78 -17.15 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.54 -27.70 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.65 -3.56 -2.91 O2

Initial solution 56. 30/8/2012 01:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.433e-004 5.433e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.270

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 317

Density (g/cm3) = 0.99653

Activity of water = 1.000

Ionic strength = 4.760e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.965e-003

Total CO2 (mol/kg) = 2.965e-003

Temperature (deg C) = 27.700

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551609e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1370 0.7245

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.458e-006 2.280e-006 -5.609 -5.642 -0.033

H+ 5.745e-009 5.370e-009 -8.241 -8.270 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.965e-003

HCO3- 2.819e-003 2.622e-003 -2.550 -2.581 -0.031

CaCO3 3.292e-005 3.296e-005 -4.483 -4.482 0.000

CO3-2 3.224e-005 2.413e-005 -4.492 -4.617 -0.126

CO2 3.065e-005 3.069e-005 -4.514 -4.513 0.000

CaHCO3+ 2.872e-005 2.671e-005 -4.542 -4.573 -0.031

MgHCO3+ 1.232e-005 1.143e-005 -4.910 -4.942 -0.032

MgCO3 8.822e-006 8.832e-006 -5.054 -5.054 0.000

NaHCO3 1.366e-008 1.368e-008 -7.865 -7.864 0.000

NaCO3- 5.138e-009 4.770e-009 -8.289 -8.321 -0.032

Ca 1.100e-003

Ca+2 1.027e-003 7.681e-004 -2.989 -3.115 -0.126

CaCO3 3.292e-005 3.296e-005 -4.483 -4.482 0.000

CaHCO3+ 2.872e-005 2.671e-005 -4.542 -4.573 -0.031

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

CaOH+ 2.557e-008 2.374e-008 -7.592 -7.625 -0.032

CaHSO4+ 4.002e-013 3.716e-013 -12.398 -12.430 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 3.972e-028

H2 1.986e-028 1.988e-028 -27.702 -27.702 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.775e-009 1.648e-009 -8.751 -8.783 -0.032

KOH 1.988e-012 1.990e-012 -11.702 -11.701 0.000

Mg 5.184e-004

Mg+2 4.902e-004 3.680e-004 -3.310 -3.434 -0.125

MgHCO3+ 1.232e-005 1.143e-005 -4.910 -4.942 -0.032

MgCO3 8.822e-006 8.832e-006 -5.054 -5.054 0.000

MgSO4 6.702e-006 6.709e-006 -5.174 -5.173 0.000

MgOH+ 3.412e-007 3.167e-007 -6.467 -6.499 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.366e-008 1.368e-008 -7.865 -7.864 0.000

NaCO3- 5.138e-009 4.770e-009 -8.289 -8.321 -0.032

NaSO4- 3.698e-009 3.433e-009 -8.432 -8.464 -0.032

NaOH 1.140e-011 1.141e-011 -10.943 -10.943 0.000

O(0) 5.433e-004

O2 2.716e-004 2.719e-004 -3.566 -3.566 0.000

S(6) 1.154e-004

SO4-2 9.727e-005 7.260e-005 -4.012 -4.139 -0.127

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

MgSO4 6.702e-006 6.709e-006 -5.174 -5.173 0.000

NaSO4- 3.698e-009 3.433e-009 -8.432 -8.464 -0.032

KSO4- 1.775e-009 1.648e-009 -8.751 -8.783 -0.032

HSO4- 4.334e-011 4.023e-011 -10.363 -10.395 -0.032

CaHSO4+ 4.002e-013 3.716e-013 -12.398 -12.430 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.62 -7.73 -8.35 CaCO3

Calcite 0.76 -7.73 -8.50 CaCO3

CO2(g) -3.01 -4.51 -1.50 CO2

Dolomite 1.37 -15.78 -17.15 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.54 -27.70 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.65 -3.57 -2.91 O2

Initial solution 57. 30/8/2012 01:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.445e-004 5.445e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.260

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 317

Density (g/cm3) = 0.99653

Activity of water = 1.000

Ionic strength = 4.761e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.967e-003

Total CO2 (mol/kg) = 2.967e-003

Temperature (deg C) = 27.700

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551609e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1472 0.7251

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.402e-006 2.228e-006 -5.619 -5.652 -0.033

H+ 5.879e-009 5.495e-009 -8.231 -8.260 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.967e-003

HCO3- 2.822e-003 2.625e-003 -2.549 -2.581 -0.031

CaCO3 3.222e-005 3.226e-005 -4.492 -4.491 0.000

CO3-2 3.154e-005 2.361e-005 -4.501 -4.627 -0.126

CO2 3.140e-005 3.144e-005 -4.503 -4.503 0.000

CaHCO3+ 2.877e-005 2.676e-005 -4.541 -4.573 -0.031

MgHCO3+ 1.233e-005 1.145e-005 -4.909 -4.941 -0.032

MgCO3 8.634e-006 8.643e-006 -5.064 -5.063 0.000

NaHCO3 1.368e-008 1.369e-008 -7.864 -7.864 0.000

NaCO3- 5.027e-009 4.667e-009 -8.299 -8.331 -0.032

Ca 1.100e-003

Ca+2 1.027e-003 7.686e-004 -2.988 -3.114 -0.126

CaCO3 3.222e-005 3.226e-005 -4.492 -4.491 0.000

CaHCO3+ 2.877e-005 2.676e-005 -4.541 -4.573 -0.031

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

CaOH+ 2.500e-008 2.321e-008 -7.602 -7.634 -0.032

CaHSO4+ 4.098e-013 3.804e-013 -12.387 -12.420 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 4.159e-028

H2 2.079e-028 2.082e-028 -27.682 -27.682 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.775e-009 1.648e-009 -8.751 -8.783 -0.032

KOH 1.943e-012 1.945e-012 -11.712 -11.711 0.000

Mg 5.184e-004

Mg+2 4.904e-004 3.681e-004 -3.309 -3.434 -0.125

MgHCO3+ 1.233e-005 1.145e-005 -4.909 -4.941 -0.032

MgCO3 8.634e-006 8.643e-006 -5.064 -5.063 0.000

MgSO4 6.703e-006 6.711e-006 -5.174 -5.173 0.000

MgOH+ 3.335e-007 3.096e-007 -6.477 -6.509 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.368e-008 1.369e-008 -7.864 -7.864 0.000

NaCO3- 5.027e-009 4.667e-009 -8.299 -8.331 -0.032

NaSO4- 3.697e-009 3.432e-009 -8.432 -8.464 -0.032

NaOH 1.114e-011 1.115e-011 -10.953 -10.953 0.000

O(0) 5.445e-004

O2 2.723e-004 2.726e-004 -3.565 -3.565 0.000

S(6) 1.154e-004

SO4-2 9.726e-005 7.259e-005 -4.012 -4.139 -0.127

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

MgSO4 6.703e-006 6.711e-006 -5.174 -5.173 0.000

NaSO4- 3.697e-009 3.432e-009 -8.432 -8.464 -0.032

KSO4- 1.775e-009 1.648e-009 -8.751 -8.783 -0.032

HSO4- 4.434e-011 4.117e-011 -10.353 -10.385 -0.032

CaHSO4+ 4.098e-013 3.804e-013 -12.387 -12.420 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.61 -7.74 -8.35 CaCO3

Calcite 0.75 -7.74 -8.50 CaCO3

CO2(g) -3.00 -4.50 -1.50 CO2

Dolomite 1.35 -15.80 -17.15 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.52 -27.68 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.65 -3.56 -2.91 O2

Initial solution 58. 30/8/2012 02:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.370e-004 5.370e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.270

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 316

Density (g/cm3) = 0.99653

Activity of water = 1.000

Ionic strength = 4.748e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.954e-003

Total CO2 (mol/kg) = 2.954e-003

Temperature (deg C) = 27.700

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551605e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1357 0.7244

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.458e-006 2.280e-006 -5.609 -5.642 -0.033

H+ 5.745e-009 5.370e-009 -8.241 -8.270 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.954e-003

HCO3- 2.809e-003 2.613e-003 -2.551 -2.583 -0.031

CaCO3 3.272e-005 3.275e-005 -4.485 -4.485 0.000

CO3-2 3.212e-005 2.405e-005 -4.493 -4.619 -0.126

CO2 3.055e-005 3.059e-005 -4.515 -4.514 0.000

CaHCO3+ 2.854e-005 2.655e-005 -4.545 -4.576 -0.031

MgHCO3+ 1.228e-005 1.140e-005 -4.911 -4.943 -0.032

MgCO3 8.797e-006 8.807e-006 -5.056 -5.055 0.000

NaHCO3 1.362e-008 1.363e-008 -7.866 -7.865 0.000

NaCO3- 5.121e-009 4.755e-009 -8.291 -8.323 -0.032

Ca 1.096e-003

Ca+2 1.023e-003 7.659e-004 -2.990 -3.116 -0.126

CaCO3 3.272e-005 3.275e-005 -4.485 -4.485 0.000

CaHCO3+ 2.854e-005 2.655e-005 -4.545 -4.576 -0.031

CaSO4 1.137e-005 1.138e-005 -4.944 -4.944 0.000

CaOH+ 2.549e-008 2.367e-008 -7.594 -7.626 -0.032

CaHSO4+ 3.992e-013 3.707e-013 -12.399 -12.431 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 3.972e-028

H2 1.986e-028 1.988e-028 -27.702 -27.702 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.776e-009 1.649e-009 -8.751 -8.783 -0.032

KOH 1.988e-012 1.991e-012 -11.701 -11.701 0.000

Mg 5.184e-004

Mg+2 4.903e-004 3.681e-004 -3.310 -3.434 -0.124

MgHCO3+ 1.228e-005 1.140e-005 -4.911 -4.943 -0.032

MgCO3 8.797e-006 8.807e-006 -5.056 -5.055 0.000

MgSO4 6.708e-006 6.716e-006 -5.173 -5.173 0.000

MgOH+ 3.413e-007 3.169e-007 -6.467 -6.499 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.362e-008 1.363e-008 -7.866 -7.865 0.000

NaCO3- 5.121e-009 4.755e-009 -8.291 -8.323 -0.032

NaSO4- 3.700e-009 3.435e-009 -8.432 -8.464 -0.032

NaOH 1.140e-011 1.141e-011 -10.943 -10.943 0.000

O(0) 5.370e-004

O2 2.685e-004 2.688e-004 -3.571 -3.571 0.000

S(6) 1.154e-004

SO4-2 9.729e-005 7.264e-005 -4.012 -4.139 -0.127

CaSO4 1.137e-005 1.138e-005 -4.944 -4.944 0.000

MgSO4 6.708e-006 6.716e-006 -5.173 -5.173 0.000

NaSO4- 3.700e-009 3.435e-009 -8.432 -8.464 -0.032

KSO4- 1.776e-009 1.649e-009 -8.751 -8.783 -0.032

HSO4- 4.336e-011 4.026e-011 -10.363 -10.395 -0.032

CaHSO4+ 3.992e-013 3.707e-013 -12.399 -12.431 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.62 -7.73 -8.35 CaCO3

Calcite 0.76 -7.73 -8.50 CaCO3

CO2(g) -3.02 -4.51 -1.50 CO2

Dolomite 1.36 -15.79 -17.15 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.54 -27.70 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.66 -3.57 -2.91 O2

Initial solution 59. 30/8/2012 02:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.326e-004 5.326e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.260

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 316

Density (g/cm3) = 0.99656

Activity of water = 1.000

Ionic strength = 4.762e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.967e-003

Total CO2 (mol/kg) = 2.967e-003

Temperature (deg C) = 27.600

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551608e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1530 0.7252

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.385e-006 2.212e-006 -5.623 -5.655 -0.033

H+ 5.879e-009 5.495e-009 -8.231 -8.260 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.967e-003

HCO3- 2.822e-003 2.625e-003 -2.549 -2.581 -0.031

CaCO3 3.210e-005 3.214e-005 -4.493 -4.493 0.000

CO3-2 3.149e-005 2.357e-005 -4.502 -4.628 -0.126

CO2 3.144e-005 3.148e-005 -4.502 -4.502 0.000

CaHCO3+ 2.874e-005 2.673e-005 -4.542 -4.573 -0.031

MgHCO3+ 1.233e-005 1.145e-005 -4.909 -4.941 -0.032

MgCO3 8.607e-006 8.616e-006 -5.065 -5.065 0.000

NaHCO3 1.368e-008 1.369e-008 -7.864 -7.864 0.000

NaCO3- 4.993e-009 4.636e-009 -8.302 -8.334 -0.032

Ca 1.100e-003

Ca+2 1.028e-003 7.687e-004 -2.988 -3.114 -0.126

CaCO3 3.210e-005 3.214e-005 -4.493 -4.493 0.000

CaHCO3+ 2.874e-005 2.673e-005 -4.542 -4.573 -0.031

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

CaOH+ 2.501e-008 2.321e-008 -7.602 -7.634 -0.032

CaHSO4+ 4.090e-013 3.797e-013 -12.388 -12.421 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 4.163e-028

H2 2.082e-028 2.084e-028 -27.682 -27.681 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.772e-009 1.645e-009 -8.751 -8.784 -0.032

KOH 1.943e-012 1.945e-012 -11.712 -11.711 0.000

Mg 5.184e-004

Mg+2 4.904e-004 3.681e-004 -3.309 -3.434 -0.125

MgHCO3+ 1.233e-005 1.145e-005 -4.909 -4.941 -0.032

MgCO3 8.607e-006 8.616e-006 -5.065 -5.065 0.000

MgSO4 6.689e-006 6.696e-006 -5.175 -5.174 0.000

MgOH+ 3.306e-007 3.069e-007 -6.481 -6.513 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.368e-008 1.369e-008 -7.864 -7.864 0.000

NaCO3- 4.993e-009 4.636e-009 -8.302 -8.334 -0.032

NaSO4- 3.696e-009 3.431e-009 -8.432 -8.465 -0.032

NaOH 1.114e-011 1.115e-011 -10.953 -10.953 0.000

O(0) 5.326e-004

O2 2.663e-004 2.666e-004 -3.575 -3.574 0.000

S(6) 1.154e-004

SO4-2 9.728e-005 7.261e-005 -4.012 -4.139 -0.127

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

MgSO4 6.689e-006 6.696e-006 -5.175 -5.174 0.000

NaSO4- 3.696e-009 3.431e-009 -8.432 -8.465 -0.032

KSO4- 1.772e-009 1.645e-009 -8.751 -8.784 -0.032

HSO4- 4.426e-011 4.108e-011 -10.354 -10.386 -0.032

CaHSO4+ 4.090e-013 3.797e-013 -12.388 -12.421 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.61 -7.74 -8.35 CaCO3

Calcite 0.75 -7.74 -8.49 CaCO3

CO2(g) -3.00 -4.50 -1.50 CO2

Dolomite 1.35 -15.80 -17.15 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.52 -27.68 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.66 -3.57 -2.91 O2

Initial solution 60. 30/8/2012 02:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.364e-004 5.364e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.250

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 316

Density (g/cm3) = 0.99656

Activity of water = 1.000

Ionic strength = 4.764e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.970e-003

Total CO2 (mol/kg) = 2.970e-003

Temperature (deg C) = 27.600

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551609e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1637 0.7258

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.330e-006 2.161e-006 -5.633 -5.665 -0.033

H+ 6.016e-009 5.623e-009 -8.221 -8.250 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.970e-003

HCO3- 2.826e-003 2.628e-003 -2.549 -2.580 -0.031

CO2 3.221e-005 3.225e-005 -4.492 -4.492 0.000

CaCO3 3.143e-005 3.146e-005 -4.503 -4.502 0.000

CO3-2 3.080e-005 2.306e-005 -4.511 -4.637 -0.126

CaHCO3+ 2.879e-005 2.678e-005 -4.541 -4.572 -0.031

MgHCO3+ 1.235e-005 1.146e-005 -4.908 -4.941 -0.032

MgCO3 8.422e-006 8.432e-006 -5.075 -5.074 0.000

NaHCO3 1.369e-008 1.371e-008 -7.864 -7.863 0.000

NaCO3- 4.885e-009 4.535e-009 -8.311 -8.343 -0.032

Ca 1.100e-003

Ca+2 1.028e-003 7.692e-004 -2.988 -3.114 -0.126

CaCO3 3.143e-005 3.146e-005 -4.503 -4.502 0.000

CaHCO3+ 2.879e-005 2.678e-005 -4.541 -4.572 -0.031

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

CaOH+ 2.445e-008 2.270e-008 -7.612 -7.644 -0.032

CaHSO4+ 4.187e-013 3.887e-013 -12.378 -12.410 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 4.359e-028

H2 2.180e-028 2.182e-028 -27.662 -27.661 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.772e-009 1.645e-009 -8.751 -8.784 -0.032

KOH 1.899e-012 1.901e-012 -11.722 -11.721 0.000

Mg 5.184e-004

Mg+2 4.906e-004 3.682e-004 -3.309 -3.434 -0.125

MgHCO3+ 1.235e-005 1.146e-005 -4.908 -4.941 -0.032

MgCO3 8.422e-006 8.432e-006 -5.075 -5.074 0.000

MgSO4 6.690e-006 6.697e-006 -5.175 -5.174 0.000

MgOH+ 3.232e-007 3.000e-007 -6.491 -6.523 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.369e-008 1.371e-008 -7.864 -7.863 0.000

NaCO3- 4.885e-009 4.535e-009 -8.311 -8.343 -0.032

NaSO4- 3.695e-009 3.431e-009 -8.432 -8.465 -0.032

NaOH 1.088e-011 1.090e-011 -10.963 -10.963 0.000

O(0) 5.364e-004

O2 2.682e-004 2.685e-004 -3.572 -3.571 0.000

S(6) 1.154e-004

SO4-2 9.727e-005 7.260e-005 -4.012 -4.139 -0.127

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

MgSO4 6.690e-006 6.697e-006 -5.175 -5.174 0.000

NaSO4- 3.695e-009 3.431e-009 -8.432 -8.465 -0.032

KSO4- 1.772e-009 1.645e-009 -8.751 -8.784 -0.032

HSO4- 4.528e-011 4.204e-011 -10.344 -10.376 -0.032

CaHSO4+ 4.187e-013 3.887e-013 -12.378 -12.410 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.60 -7.75 -8.35 CaCO3

Calcite 0.74 -7.75 -8.49 CaCO3

CO2(g) -2.99 -4.49 -1.50 CO2

Dolomite 1.33 -15.82 -17.15 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.50 -27.66 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.66 -3.57 -2.91 O2

Initial solution 61. 30/8/2012 02:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.258e-004 5.258e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.220

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 316

Density (g/cm3) = 0.99659

Activity of water = 1.000

Ionic strength = 4.769e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.977e-003

Total CO2 (mol/kg) = 2.977e-003

Temperature (deg C) = 27.500

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551610e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1997 0.7277

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.159e-006 2.002e-006 -5.666 -5.699 -0.033

H+ 6.447e-009 6.026e-009 -8.191 -8.220 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.977e-003

HCO3- 2.835e-003 2.637e-003 -2.547 -2.579 -0.031

CO2 3.466e-005 3.470e-005 -4.460 -4.460 0.000

CaCO3 2.936e-005 2.939e-005 -4.532 -4.532 0.000

CaHCO3+ 2.889e-005 2.687e-005 -4.539 -4.571 -0.031

CO3-2 2.879e-005 2.155e-005 -4.541 -4.667 -0.126

MgHCO3+ 1.240e-005 1.151e-005 -4.907 -4.939 -0.032

MgCO3 7.867e-006 7.876e-006 -5.104 -5.104 0.000

NaHCO3 1.374e-008 1.375e-008 -7.862 -7.862 0.000

NaCO3- 4.543e-009 4.217e-009 -8.343 -8.375 -0.032

Ca 1.100e-003

Ca+2 1.030e-003 7.705e-004 -2.987 -3.113 -0.126

CaCO3 2.936e-005 2.939e-005 -4.532 -4.532 0.000

CaHCO3+ 2.889e-005 2.687e-005 -4.539 -4.571 -0.031

CaSO4 1.141e-005 1.142e-005 -4.943 -4.942 0.000

CaOH+ 2.286e-008 2.122e-008 -7.641 -7.673 -0.032

CaHSO4+ 4.485e-013 4.163e-013 -12.348 -12.381 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 5.010e-028

H2 2.505e-028 2.508e-028 -27.601 -27.601 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.769e-009 1.642e-009 -8.752 -8.785 -0.032

KOH 1.772e-012 1.774e-012 -11.752 -11.751 0.000

Mg 5.184e-004

Mg+2 4.912e-004 3.686e-004 -3.309 -3.433 -0.125

MgHCO3+ 1.240e-005 1.151e-005 -4.907 -4.939 -0.032

MgCO3 7.867e-006 7.876e-006 -5.104 -5.104 0.000

MgSO4 6.679e-006 6.687e-006 -5.175 -5.175 0.000

MgOH+ 2.993e-007 2.778e-007 -6.524 -6.556 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.374e-008 1.375e-008 -7.862 -7.862 0.000

NaCO3- 4.543e-009 4.217e-009 -8.343 -8.375 -0.032

NaSO4- 3.693e-009 3.428e-009 -8.433 -8.465 -0.032

NaOH 1.016e-011 1.017e-011 -10.993 -10.993 0.000

O(0) 5.258e-004

O2 2.629e-004 2.632e-004 -3.580 -3.580 0.000

S(6) 1.154e-004

SO4-2 9.728e-005 7.260e-005 -4.012 -4.139 -0.127

CaSO4 1.141e-005 1.142e-005 -4.943 -4.942 0.000

MgSO4 6.679e-006 6.687e-006 -5.175 -5.175 0.000

NaSO4- 3.693e-009 3.428e-009 -8.433 -8.465 -0.032

KSO4- 1.769e-009 1.642e-009 -8.752 -8.785 -0.032

HSO4- 4.841e-011 4.494e-011 -10.315 -10.347 -0.032

CaHSO4+ 4.485e-013 4.163e-013 -12.348 -12.381 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.57 -7.78 -8.35 CaCO3

Calcite 0.71 -7.78 -8.49 CaCO3

CO2(g) -2.96 -4.46 -1.50 CO2

Dolomite 1.27 -15.88 -17.15 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.44 -27.60 -3.16 H2

H2O(g) -1.45 -0.00 1.45 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.67 -3.58 -2.91 O2

Initial solution 62. 30/8/2012 03:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.183e-004 5.183e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.220

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 315

Density (g/cm3) = 0.99659

Activity of water = 1.000

Ionic strength = 4.758e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.967e-003

Total CO2 (mol/kg) = 2.967e-003

Temperature (deg C) = 27.500

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551606e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1981 0.7276

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.159e-006 2.002e-006 -5.666 -5.699 -0.033

H+ 6.446e-009 6.026e-009 -8.191 -8.220 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.967e-003

HCO3- 2.825e-003 2.628e-003 -2.549 -2.580 -0.031

CO2 3.455e-005 3.459e-005 -4.462 -4.461 0.000

CaCO3 2.918e-005 2.921e-005 -4.535 -4.535 0.000

CaHCO3+ 2.871e-005 2.671e-005 -4.542 -4.573 -0.031

CO3-2 2.869e-005 2.148e-005 -4.542 -4.668 -0.126

MgHCO3+ 1.236e-005 1.147e-005 -4.908 -4.940 -0.032

MgCO3 7.844e-006 7.853e-006 -5.105 -5.105 0.000

NaHCO3 1.369e-008 1.371e-008 -7.863 -7.863 0.000

NaCO3- 4.528e-009 4.204e-009 -8.344 -8.376 -0.032

Ca 1.096e-003

Ca+2 1.027e-003 7.683e-004 -2.989 -3.114 -0.126

CaCO3 2.918e-005 2.921e-005 -4.535 -4.535 0.000

CaHCO3+ 2.871e-005 2.671e-005 -4.542 -4.573 -0.031

CaSO4 1.138e-005 1.140e-005 -4.944 -4.943 0.000

CaOH+ 2.279e-008 2.116e-008 -7.642 -7.675 -0.032

CaHSO4+ 4.473e-013 4.153e-013 -12.349 -12.382 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 5.010e-028

H2 2.505e-028 2.508e-028 -27.601 -27.601 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.770e-009 1.643e-009 -8.752 -8.784 -0.032

KOH 1.772e-012 1.774e-012 -11.752 -11.751 0.000

Mg 5.184e-004

Mg+2 4.912e-004 3.688e-004 -3.309 -3.433 -0.125

MgHCO3+ 1.236e-005 1.147e-005 -4.908 -4.940 -0.032

MgCO3 7.844e-006 7.853e-006 -5.105 -5.105 0.000

MgSO4 6.686e-006 6.693e-006 -5.175 -5.174 0.000

MgOH+ 2.994e-007 2.779e-007 -6.524 -6.556 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.369e-008 1.371e-008 -7.863 -7.863 0.000

NaCO3- 4.528e-009 4.204e-009 -8.344 -8.376 -0.032

NaSO4- 3.695e-009 3.430e-009 -8.432 -8.465 -0.032

NaOH 1.016e-011 1.017e-011 -10.993 -10.993 0.000

O(0) 5.183e-004

O2 2.591e-004 2.594e-004 -3.586 -3.586 0.000

S(6) 1.154e-004

SO4-2 9.730e-005 7.264e-005 -4.012 -4.139 -0.127

CaSO4 1.138e-005 1.140e-005 -4.944 -4.943 0.000

MgSO4 6.686e-006 6.693e-006 -5.175 -5.174 0.000

NaSO4- 3.695e-009 3.430e-009 -8.432 -8.465 -0.032

KSO4- 1.770e-009 1.643e-009 -8.752 -8.784 -0.032

HSO4- 4.843e-011 4.496e-011 -10.315 -10.347 -0.032

CaHSO4+ 4.473e-013 4.153e-013 -12.349 -12.382 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.57 -7.78 -8.35 CaCO3

Calcite 0.71 -7.78 -8.49 CaCO3

CO2(g) -2.96 -4.46 -1.50 CO2

Dolomite 1.26 -15.88 -17.15 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.44 -27.60 -3.16 H2

H2O(g) -1.45 -0.00 1.45 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.68 -3.59 -2.91 O2

Initial solution 63. 30/8/2012 03:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.133e-004 5.133e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.230

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 315

Density (g/cm3) = 0.99662

Activity of water = 1.000

Ionic strength = 4.768e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.975e-003

Total CO2 (mol/kg) = 2.975e-003

Temperature (deg C) = 27.400

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551608e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1952 0.7272

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.193e-006 2.034e-006 -5.659 -5.692 -0.033

H+ 6.300e-009 5.888e-009 -8.201 -8.230 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.975e-003

HCO3- 2.832e-003 2.634e-003 -2.548 -2.579 -0.031

CO2 3.388e-005 3.392e-005 -4.470 -4.470 0.000

CaCO3 2.988e-005 2.992e-005 -4.525 -4.524 0.000

CO3-2 2.938e-005 2.199e-005 -4.532 -4.658 -0.126

CaHCO3+ 2.882e-005 2.681e-005 -4.540 -4.572 -0.031

MgHCO3+ 1.238e-005 1.149e-005 -4.907 -4.940 -0.032

MgCO3 8.015e-006 8.023e-006 -5.096 -5.096 0.000

NaHCO3 1.373e-008 1.374e-008 -7.862 -7.862 0.000

NaCO3- 4.613e-009 4.282e-009 -8.336 -8.368 -0.032

Ca 1.100e-003

Ca+2 1.030e-003 7.703e-004 -2.987 -3.113 -0.126

CaCO3 2.988e-005 2.992e-005 -4.525 -4.524 0.000

CaHCO3+ 2.882e-005 2.681e-005 -4.540 -4.572 -0.031

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

CaOH+ 2.338e-008 2.171e-008 -7.631 -7.663 -0.032

CaHSO4+ 4.373e-013 4.059e-013 -12.359 -12.392 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 4.789e-028

H2 2.395e-028 2.397e-028 -27.621 -27.620 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.767e-009 1.640e-009 -8.753 -8.785 -0.032

KOH 1.813e-012 1.815e-012 -11.742 -11.741 0.000

Mg 5.184e-004

Mg+2 4.910e-004 3.685e-004 -3.309 -3.434 -0.125

MgHCO3+ 1.238e-005 1.149e-005 -4.907 -4.940 -0.032

MgCO3 8.015e-006 8.023e-006 -5.096 -5.096 0.000

MgSO4 6.664e-006 6.671e-006 -5.176 -5.176 0.000

MgOH+ 3.035e-007 2.817e-007 -6.518 -6.550 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.373e-008 1.374e-008 -7.862 -7.862 0.000

NaCO3- 4.613e-009 4.282e-009 -8.336 -8.368 -0.032

NaSO4- 3.692e-009 3.427e-009 -8.433 -8.465 -0.032

NaOH 1.039e-011 1.041e-011 -10.983 -10.983 0.000

O(0) 5.133e-004

O2 2.566e-004 2.569e-004 -3.591 -3.590 0.000

S(6) 1.154e-004

SO4-2 9.730e-005 7.262e-005 -4.012 -4.139 -0.127

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

MgSO4 6.664e-006 6.671e-006 -5.176 -5.176 0.000

NaSO4- 3.692e-009 3.427e-009 -8.433 -8.465 -0.032

KSO4- 1.767e-009 1.640e-009 -8.753 -8.785 -0.032

HSO4- 4.722e-011 4.383e-011 -10.326 -10.358 -0.032

CaHSO4+ 4.373e-013 4.059e-013 -12.359 -12.392 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.58 -7.77 -8.35 CaCO3

Calcite 0.72 -7.77 -8.49 CaCO3

CO2(g) -2.97 -4.47 -1.50 CO2

Dolomite 1.28 -15.86 -17.15 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.46 -27.62 -3.16 H2

H2O(g) -1.45 -0.00 1.45 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.68 -3.59 -2.91 O2

Initial solution 64. 30/8/2012 03:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.151e-004 5.151e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.210

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 315

Density (g/cm3) = 0.99662

Activity of water = 1.000

Ionic strength = 4.771e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.979e-003

Total CO2 (mol/kg) = 2.979e-003

Temperature (deg C) = 27.400

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551610e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.2156 0.7284

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.094e-006 1.942e-006 -5.679 -5.712 -0.033

H+ 6.597e-009 6.166e-009 -8.181 -8.210 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.979e-003

HCO3- 2.838e-003 2.640e-003 -2.547 -2.578 -0.031

CO2 3.555e-005 3.559e-005 -4.449 -4.449 0.000

CaHCO3+ 2.891e-005 2.689e-005 -4.539 -4.570 -0.031

CaCO3 2.863e-005 2.866e-005 -4.543 -4.543 0.000

CO3-2 2.812e-005 2.104e-005 -4.551 -4.677 -0.126

MgHCO3+ 1.241e-005 1.152e-005 -4.906 -4.939 -0.032

MgCO3 7.673e-006 7.682e-006 -5.115 -5.115 0.000

NaHCO3 1.375e-008 1.377e-008 -7.862 -7.861 0.000

NaCO3- 4.414e-009 4.098e-009 -8.355 -8.387 -0.032

Ca 1.100e-003

Ca+2 1.031e-003 7.711e-004 -2.987 -3.113 -0.126

CaHCO3+ 2.891e-005 2.689e-005 -4.539 -4.570 -0.031

CaCO3 2.863e-005 2.866e-005 -4.543 -4.543 0.000

CaSO4 1.141e-005 1.142e-005 -4.943 -4.942 0.000

CaOH+ 2.235e-008 2.075e-008 -7.651 -7.683 -0.032

CaHSO4+ 4.583e-013 4.254e-013 -12.339 -12.371 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 5.251e-028

H2 2.626e-028 2.628e-028 -27.581 -27.580 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.766e-009 1.640e-009 -8.753 -8.785 -0.032

KOH 1.732e-012 1.734e-012 -11.762 -11.761 0.000

Mg 5.184e-004

Mg+2 4.914e-004 3.688e-004 -3.309 -3.433 -0.125

MgHCO3+ 1.241e-005 1.152e-005 -4.906 -4.939 -0.032

MgCO3 7.673e-006 7.682e-006 -5.115 -5.115 0.000

MgSO4 6.666e-006 6.673e-006 -5.176 -5.176 0.000

MgOH+ 2.900e-007 2.692e-007 -6.538 -6.570 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.375e-008 1.377e-008 -7.862 -7.861 0.000

NaCO3- 4.414e-009 4.098e-009 -8.355 -8.387 -0.032

NaSO4- 3.691e-009 3.427e-009 -8.433 -8.465 -0.032

NaOH 9.927e-012 9.938e-012 -11.003 -11.003 0.000

O(0) 5.151e-004

O2 2.576e-004 2.579e-004 -3.589 -3.589 0.000

S(6) 1.154e-004

SO4-2 9.729e-005 7.261e-005 -4.012 -4.139 -0.127

CaSO4 1.141e-005 1.142e-005 -4.943 -4.942 0.000

MgSO4 6.666e-006 6.673e-006 -5.176 -5.176 0.000

NaSO4- 3.691e-009 3.427e-009 -8.433 -8.465 -0.032

KSO4- 1.766e-009 1.640e-009 -8.753 -8.785 -0.032

HSO4- 4.943e-011 4.589e-011 -10.306 -10.338 -0.032

CaHSO4+ 4.583e-013 4.254e-013 -12.339 -12.371 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.56 -7.79 -8.35 CaCO3

Calcite 0.70 -7.79 -8.49 CaCO3

CO2(g) -2.95 -4.45 -1.50 CO2

Dolomite 1.25 -15.90 -17.15 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.42 -27.58 -3.16 H2

H2O(g) -1.45 -0.00 1.45 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.68 -3.59 -2.91 O2

Initial solution 65. 30/8/2012 03:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.126e-004 5.126e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.200

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 315

Density (g/cm3) = 0.99662

Activity of water = 1.000

Ionic strength = 4.773e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.982e-003

Total CO2 (mol/kg) = 2.982e-003

Temperature (deg C) = 27.400

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551610e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.2251 0.7290

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.047e-006 1.898e-006 -5.689 -5.722 -0.033

H+ 6.751e-009 6.310e-009 -8.171 -8.200 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.982e-003

HCO3- 2.841e-003 2.642e-003 -2.547 -2.578 -0.031

CO2 3.641e-005 3.645e-005 -4.439 -4.438 0.000

CaHCO3+ 2.895e-005 2.693e-005 -4.538 -4.570 -0.031

CaCO3 2.801e-005 2.805e-005 -4.553 -4.552 0.000

CO3-2 2.750e-005 2.058e-005 -4.561 -4.687 -0.126

MgHCO3+ 1.242e-005 1.153e-005 -4.906 -4.938 -0.032

MgCO3 7.508e-006 7.516e-006 -5.124 -5.124 0.000

NaHCO3 1.377e-008 1.378e-008 -7.861 -7.861 0.000

NaCO3- 4.318e-009 4.008e-009 -8.365 -8.397 -0.032

Ca 1.100e-003

Ca+2 1.031e-003 7.715e-004 -2.987 -3.113 -0.126

CaHCO3+ 2.895e-005 2.693e-005 -4.538 -4.570 -0.031

CaCO3 2.801e-005 2.805e-005 -4.553 -4.552 0.000

CaSO4 1.141e-005 1.143e-005 -4.943 -4.942 0.000

CaOH+ 2.186e-008 2.029e-008 -7.660 -7.693 -0.032

CaHSO4+ 4.691e-013 4.355e-013 -12.329 -12.361 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 5.499e-028

H2 2.749e-028 2.752e-028 -27.561 -27.560 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.766e-009 1.639e-009 -8.753 -8.785 -0.032

KOH 1.692e-012 1.694e-012 -11.772 -11.771 0.000

Mg 5.184e-004

Mg+2 4.915e-004 3.689e-004 -3.308 -3.433 -0.125

MgHCO3+ 1.242e-005 1.153e-005 -4.906 -4.938 -0.032

MgCO3 7.508e-006 7.516e-006 -5.124 -5.124 0.000

MgSO4 6.667e-006 6.674e-006 -5.176 -5.176 0.000

MgOH+ 2.835e-007 2.631e-007 -6.547 -6.580 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.377e-008 1.378e-008 -7.861 -7.861 0.000

NaCO3- 4.318e-009 4.008e-009 -8.365 -8.397 -0.032

NaSO4- 3.691e-009 3.426e-009 -8.433 -8.465 -0.032

NaOH 9.701e-012 9.712e-012 -11.013 -11.013 0.000

O(0) 5.126e-004

O2 2.563e-004 2.566e-004 -3.591 -3.591 0.000

S(6) 1.154e-004

SO4-2 9.728e-005 7.260e-005 -4.012 -4.139 -0.127

CaSO4 1.141e-005 1.143e-005 -4.943 -4.942 0.000

MgSO4 6.667e-006 6.674e-006 -5.176 -5.176 0.000

NaSO4- 3.691e-009 3.426e-009 -8.433 -8.465 -0.032

KSO4- 1.766e-009 1.639e-009 -8.753 -8.785 -0.032

HSO4- 5.058e-011 4.695e-011 -10.296 -10.328 -0.032

CaHSO4+ 4.691e-013 4.355e-013 -12.329 -12.361 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.55 -7.80 -8.35 CaCO3

Calcite 0.69 -7.80 -8.49 CaCO3

CO2(g) -2.94 -4.44 -1.50 CO2

Dolomite 1.23 -15.92 -17.15 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.40 -27.56 -3.16 H2

H2O(g) -1.45 -0.00 1.45 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.68 -3.59 -2.91 O2

Initial solution 66. 30/8/2012 04:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.289e-004 5.289e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.230

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 314

Density (g/cm3) = 0.99664

Activity of water = 1.000

Ionic strength = 4.769e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.975e-003

Total CO2 (mol/kg) = 2.975e-003

Temperature (deg C) = 27.300

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551610e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.2066 0.7277

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.177e-006 2.019e-006 -5.662 -5.695 -0.033

H+ 6.300e-009 5.888e-009 -8.201 -8.230 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.975e-003

HCO3- 2.833e-003 2.635e-003 -2.548 -2.579 -0.031

CO2 3.393e-005 3.396e-005 -4.469 -4.469 0.000

CaCO3 2.977e-005 2.981e-005 -4.526 -4.526 0.000

CO3-2 2.933e-005 2.195e-005 -4.533 -4.659 -0.126

CaHCO3+ 2.879e-005 2.678e-005 -4.541 -4.572 -0.031

MgHCO3+ 1.237e-005 1.149e-005 -4.908 -4.940 -0.032

MgCO3 7.989e-006 7.998e-006 -5.097 -5.097 0.000

NaHCO3 1.373e-008 1.374e-008 -7.862 -7.862 0.000

NaCO3- 4.582e-009 4.254e-009 -8.339 -8.371 -0.032

Ca 1.100e-003

Ca+2 1.030e-003 7.704e-004 -2.987 -3.113 -0.126

CaCO3 2.977e-005 2.981e-005 -4.526 -4.526 0.000

CaHCO3+ 2.879e-005 2.678e-005 -4.541 -4.572 -0.031

CaSO4 1.139e-005 1.141e-005 -4.943 -4.943 0.000

CaOH+ 2.339e-008 2.171e-008 -7.631 -7.663 -0.032

CaHSO4+ 4.365e-013 4.052e-013 -12.360 -12.392 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 4.794e-028

H2 2.397e-028 2.400e-028 -27.620 -27.620 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.764e-009 1.638e-009 -8.754 -8.786 -0.032

KOH 1.813e-012 1.815e-012 -11.742 -11.741 0.000

Mg 5.184e-004

Mg+2 4.911e-004 3.686e-004 -3.309 -3.433 -0.125

MgHCO3+ 1.237e-005 1.149e-005 -4.908 -4.940 -0.032

MgCO3 7.989e-006 7.998e-006 -5.097 -5.097 0.000

MgSO4 6.649e-006 6.657e-006 -5.177 -5.177 0.000

MgOH+ 3.008e-007 2.793e-007 -6.522 -6.554 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.373e-008 1.374e-008 -7.862 -7.862 0.000

NaCO3- 4.582e-009 4.254e-009 -8.339 -8.371 -0.032

NaSO4- 3.691e-009 3.426e-009 -8.433 -8.465 -0.032

NaOH 1.039e-011 1.041e-011 -10.983 -10.983 0.000

O(0) 5.289e-004

O2 2.644e-004 2.647e-004 -3.578 -3.577 0.000

S(6) 1.154e-004

SO4-2 9.732e-005 7.264e-005 -4.012 -4.139 -0.127

CaSO4 1.139e-005 1.141e-005 -4.943 -4.943 0.000

MgSO4 6.649e-006 6.657e-006 -5.177 -5.177 0.000

NaSO4- 3.691e-009 3.426e-009 -8.433 -8.465 -0.032

KSO4- 1.764e-009 1.638e-009 -8.754 -8.786 -0.032

HSO4- 4.712e-011 4.375e-011 -10.327 -10.359 -0.032

CaHSO4+ 4.365e-013 4.052e-013 -12.360 -12.392 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.58 -7.77 -8.35 CaCO3

Calcite 0.72 -7.77 -8.49 CaCO3

CO2(g) -2.97 -4.47 -1.49 CO2

Dolomite 1.28 -15.86 -17.14 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.46 -27.62 -3.16 H2

H2O(g) -1.45 -0.00 1.45 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.67 -3.58 -2.91 O2

Initial solution 67. 30/8/2012 04:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.980e-003 2.980e-003

Ca 1.089e-003 1.089e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.220e-004 5.220e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.190

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 312

Density (g/cm3) = 0.99664

Activity of water = 1.000

Ionic strength = 4.740e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.954e-003

Total CO2 (mol/kg) = 2.954e-003

Temperature (deg C) = 27.300

Electrical balance (eq) = -4.035e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.65

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551603e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.2452 0.7300

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.985e-006 1.841e-006 -5.702 -5.735 -0.033

H+ 6.906e-009 6.457e-009 -8.161 -8.190 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.954e-003

HCO3- 2.815e-003 2.619e-003 -2.550 -2.582 -0.031

CO2 3.698e-005 3.702e-005 -4.432 -4.432 0.000

CaHCO3+ 2.842e-005 2.644e-005 -4.546 -4.578 -0.031

CaCO3 2.681e-005 2.684e-005 -4.572 -4.571 0.000

CO3-2 2.657e-005 1.990e-005 -4.576 -4.701 -0.125

MgHCO3+ 1.233e-005 1.145e-005 -4.909 -4.941 -0.032

MgCO3 7.260e-006 7.268e-006 -5.139 -5.139 0.000

NaHCO3 1.365e-008 1.367e-008 -7.865 -7.864 0.000

NaCO3- 4.154e-009 3.857e-009 -8.382 -8.414 -0.032

Ca 1.089e-003

Ca+2 1.022e-003 7.651e-004 -2.991 -3.116 -0.126

CaHCO3+ 2.842e-005 2.644e-005 -4.546 -4.578 -0.031

CaCO3 2.681e-005 2.684e-005 -4.572 -4.571 0.000

CaSO4 1.133e-005 1.134e-005 -4.946 -4.945 0.000

CaOH+ 2.118e-008 1.967e-008 -7.674 -7.706 -0.032

CaHSO4+ 4.758e-013 4.418e-013 -12.323 -12.355 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 5.763e-028

H2 2.882e-028 2.885e-028 -27.540 -27.540 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.766e-009 1.640e-009 -8.753 -8.785 -0.032

KOH 1.654e-012 1.656e-012 -11.781 -11.781 0.000

Mg 5.184e-004

Mg+2 4.919e-004 3.695e-004 -3.308 -3.432 -0.124

MgHCO3+ 1.233e-005 1.145e-005 -4.909 -4.941 -0.032

MgCO3 7.260e-006 7.268e-006 -5.139 -5.139 0.000

MgSO4 6.673e-006 6.680e-006 -5.176 -5.175 0.000

MgOH+ 2.749e-007 2.553e-007 -6.561 -6.593 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.278e-006 -5.001 -5.033 -0.032

NaHCO3 1.365e-008 1.367e-008 -7.865 -7.864 0.000

NaCO3- 4.154e-009 3.857e-009 -8.382 -8.414 -0.032

NaSO4- 3.695e-009 3.431e-009 -8.432 -8.465 -0.032

NaOH 9.483e-012 9.493e-012 -11.023 -11.023 0.000

O(0) 5.220e-004

O2 2.610e-004 2.613e-004 -3.583 -3.583 0.000

S(6) 1.154e-004

SO4-2 9.736e-005 7.273e-005 -4.012 -4.138 -0.127

CaSO4 1.133e-005 1.134e-005 -4.946 -4.945 0.000

MgSO4 6.673e-006 6.680e-006 -5.176 -5.175 0.000

NaSO4- 3.695e-009 3.431e-009 -8.432 -8.465 -0.032

KSO4- 1.766e-009 1.640e-009 -8.753 -8.785 -0.032

HSO4- 5.172e-011 4.803e-011 -10.286 -10.319 -0.032

CaHSO4+ 4.758e-013 4.418e-013 -12.323 -12.355 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.53 -7.82 -8.35 CaCO3

Calcite 0.68 -7.82 -8.49 CaCO3

CO2(g) -2.94 -4.43 -1.49 CO2

Dolomite 1.19 -15.95 -17.14 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.38 -27.54 -3.16 H2

H2O(g) -1.45 -0.00 1.45 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.67 -3.58 -2.91 O2

Initial solution 68. 30/8/2012 04:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.283e-004 5.283e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.180

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 314

Density (g/cm3) = 0.99667

Activity of water = 1.000

Ionic strength = 4.777e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.987e-003

Total CO2 (mol/kg) = 2.987e-003

Temperature (deg C) = 27.200

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551613e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.2647 0.7309

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.926e-006 1.786e-006 -5.715 -5.748 -0.033

H+ 7.069e-009 6.607e-009 -8.151 -8.180 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.987e-003

HCO3- 2.847e-003 2.648e-003 -2.546 -2.577 -0.031

CO2 3.830e-005 3.834e-005 -4.417 -4.416 0.000

CaHCO3+ 2.897e-005 2.695e-005 -4.538 -4.570 -0.031

CaCO3 2.663e-005 2.666e-005 -4.575 -4.574 0.000

CO3-2 2.622e-005 1.962e-005 -4.581 -4.707 -0.126

MgHCO3+ 1.245e-005 1.156e-005 -4.905 -4.937 -0.032

MgCO3 7.142e-006 7.150e-006 -5.146 -5.146 0.000

NaHCO3 1.380e-008 1.381e-008 -7.860 -7.860 0.000

NaCO3- 4.076e-009 3.784e-009 -8.390 -8.422 -0.032

Ca 1.100e-003

Ca+2 1.033e-003 7.725e-004 -2.986 -3.112 -0.126

CaHCO3+ 2.897e-005 2.695e-005 -4.538 -4.570 -0.031

CaCO3 2.663e-005 2.666e-005 -4.575 -4.574 0.000

CaSO4 1.141e-005 1.142e-005 -4.943 -4.942 0.000

CaOH+ 2.090e-008 1.940e-008 -7.680 -7.712 -0.032

CaHSO4+ 4.899e-013 4.547e-013 -12.310 -12.342 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 6.041e-028

H2 3.020e-028 3.024e-028 -27.520 -27.519 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.760e-009 1.634e-009 -8.754 -8.787 -0.032

KOH 1.616e-012 1.618e-012 -11.792 -11.791 0.000

Mg 5.184e-004

Mg+2 4.919e-004 3.691e-004 -3.308 -3.433 -0.125

MgHCO3+ 1.245e-005 1.156e-005 -4.905 -4.937 -0.032

MgCO3 7.142e-006 7.150e-006 -5.146 -5.146 0.000

MgSO4 6.640e-006 6.648e-006 -5.178 -5.177 0.000

MgOH+ 2.661e-007 2.471e-007 -6.575 -6.607 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.380e-008 1.381e-008 -7.860 -7.860 0.000

NaCO3- 4.076e-009 3.784e-009 -8.390 -8.422 -0.032

NaSO4- 3.687e-009 3.423e-009 -8.433 -8.466 -0.032

NaOH 9.264e-012 9.275e-012 -11.033 -11.033 0.000

O(0) 5.283e-004

O2 2.641e-004 2.644e-004 -3.578 -3.578 0.000

S(6) 1.154e-004

SO4-2 9.731e-005 7.262e-005 -4.012 -4.139 -0.127

CaSO4 1.141e-005 1.142e-005 -4.943 -4.942 0.000

MgSO4 6.640e-006 6.648e-006 -5.178 -5.177 0.000

NaSO4- 3.687e-009 3.423e-009 -8.433 -8.466 -0.032

KSO4- 1.760e-009 1.634e-009 -8.754 -8.787 -0.032

HSO4- 5.275e-011 4.896e-011 -10.278 -10.310 -0.032

CaHSO4+ 4.899e-013 4.547e-013 -12.310 -12.342 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.53 -7.82 -8.35 CaCO3

Calcite 0.67 -7.82 -8.49 CaCO3

CO2(g) -2.92 -4.42 -1.49 CO2

Dolomite 1.18 -15.96 -17.14 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.36 -27.52 -3.16 H2

H2O(g) -1.45 -0.00 1.45 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.67 -3.58 -2.91 O2

Initial solution 69. 30/8/2012 04:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.126e-004 5.126e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.170

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 313

Density (g/cm3) = 0.99670

Activity of water = 1.000

Ionic strength = 4.767e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.979e-003

Total CO2 (mol/kg) = 2.979e-003

Temperature (deg C) = 27.100

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551609e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.2796 0.7315

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.868e-006 1.732e-006 -5.729 -5.761 -0.033

H+ 7.233e-009 6.761e-009 -8.141 -8.170 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.979e-003

HCO3- 2.840e-003 2.642e-003 -2.547 -2.578 -0.031

CO2 3.914e-005 3.919e-005 -4.407 -4.407 0.000

CaHCO3+ 2.880e-005 2.679e-005 -4.541 -4.572 -0.031

CaCO3 2.580e-005 2.583e-005 -4.588 -4.588 0.000

CO3-2 2.551e-005 1.910e-005 -4.593 -4.719 -0.126

MgHCO3+ 1.242e-005 1.153e-005 -4.906 -4.938 -0.032

MgCO3 6.945e-006 6.953e-006 -5.158 -5.158 0.000

NaHCO3 1.377e-008 1.378e-008 -7.861 -7.861 0.000

NaCO3- 3.947e-009 3.665e-009 -8.404 -8.436 -0.032

Ca 1.096e-003

Ca+2 1.030e-003 7.707e-004 -2.987 -3.113 -0.126

CaHCO3+ 2.880e-005 2.679e-005 -4.541 -4.572 -0.031

CaCO3 2.580e-005 2.583e-005 -4.588 -4.588 0.000

CaSO4 1.138e-005 1.139e-005 -4.944 -4.943 0.000

CaOH+ 2.038e-008 1.892e-008 -7.691 -7.723 -0.032

CaHSO4+ 4.993e-013 4.635e-013 -12.302 -12.334 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 6.332e-028

H2 3.166e-028 3.169e-028 -27.499 -27.499 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.759e-009 1.633e-009 -8.755 -8.787 -0.032

KOH 1.579e-012 1.581e-012 -11.802 -11.801 0.000

Mg 5.184e-004

Mg+2 4.921e-004 3.694e-004 -3.308 -3.432 -0.125

MgHCO3+ 1.242e-005 1.153e-005 -4.906 -4.938 -0.032

MgCO3 6.945e-006 6.953e-006 -5.158 -5.158 0.000

MgSO4 6.633e-006 6.641e-006 -5.178 -5.178 0.000

MgOH+ 2.580e-007 2.395e-007 -6.588 -6.621 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.377e-008 1.378e-008 -7.861 -7.861 0.000

NaCO3- 3.947e-009 3.665e-009 -8.404 -8.436 -0.032

NaSO4- 3.688e-009 3.424e-009 -8.433 -8.466 -0.032

NaOH 9.054e-012 9.064e-012 -11.043 -11.043 0.000

O(0) 5.126e-004

O2 2.563e-004 2.566e-004 -3.591 -3.591 0.000

S(6) 1.154e-004

SO4-2 9.735e-005 7.267e-005 -4.012 -4.139 -0.127

CaSO4 1.138e-005 1.139e-005 -4.944 -4.943 0.000

MgSO4 6.633e-006 6.641e-006 -5.178 -5.178 0.000

NaSO4- 3.688e-009 3.424e-009 -8.433 -8.466 -0.032

KSO4- 1.759e-009 1.633e-009 -8.755 -8.787 -0.032

HSO4- 5.389e-011 5.003e-011 -10.269 -10.301 -0.032

CaHSO4+ 4.993e-013 4.635e-013 -12.302 -12.334 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.52 -7.83 -8.35 CaCO3

Calcite 0.66 -7.83 -8.49 CaCO3

CO2(g) -2.91 -4.41 -1.49 CO2

Dolomite 1.15 -15.98 -17.14 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.34 -27.50 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.68 -3.59 -2.91 O2

Initial solution 70. 30/8/2012 05:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.076e-004 5.076e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.140

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 314

Density (g/cm3) = 0.99670

Activity of water = 1.000

Ionic strength = 4.783e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.996e-003

Total CO2 (mol/kg) = 2.996e-003

Temperature (deg C) = 27.100

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551613e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3085 0.7333

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.743e-006 1.617e-006 -5.759 -5.791 -0.033

H+ 7.751e-009 7.244e-009 -8.111 -8.140 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.996e-003

HCO3- 2.857e-003 2.658e-003 -2.544 -2.576 -0.031

CO2 4.219e-005 4.224e-005 -4.375 -4.374 0.000

CaHCO3+ 2.909e-005 2.706e-005 -4.536 -4.568 -0.031

CaCO3 2.432e-005 2.435e-005 -4.614 -4.613 0.000

CO3-2 2.396e-005 1.793e-005 -4.621 -4.746 -0.126

MgHCO3+ 1.250e-005 1.160e-005 -4.903 -4.935 -0.032

MgCO3 6.522e-006 6.529e-006 -5.186 -5.185 0.000

NaHCO3 1.385e-008 1.386e-008 -7.859 -7.858 0.000

NaCO3- 3.706e-009 3.440e-009 -8.431 -8.463 -0.032

Ca 1.100e-003

Ca+2 1.035e-003 7.740e-004 -2.985 -3.111 -0.126

CaHCO3+ 2.909e-005 2.706e-005 -4.536 -4.568 -0.031

CaCO3 2.432e-005 2.435e-005 -4.614 -4.613 0.000

CaSO4 1.142e-005 1.143e-005 -4.942 -4.942 0.000

CaOH+ 1.910e-008 1.773e-008 -7.719 -7.751 -0.032

CaHSO4+ 5.369e-013 4.984e-013 -12.270 -12.302 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 7.270e-028

H2 3.635e-028 3.639e-028 -27.439 -27.439 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.757e-009 1.631e-009 -8.755 -8.788 -0.032

KOH 1.474e-012 1.475e-012 -11.832 -11.831 0.000

Mg 5.184e-004

Mg+2 4.925e-004 3.695e-004 -3.308 -3.432 -0.125

MgHCO3+ 1.250e-005 1.160e-005 -4.903 -4.935 -0.032

MgSO4 6.630e-006 6.637e-006 -5.178 -5.178 0.000

MgCO3 6.522e-006 6.529e-006 -5.186 -5.185 0.000

MgOH+ 2.409e-007 2.236e-007 -6.618 -6.651 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.385e-008 1.386e-008 -7.859 -7.858 0.000

NaCO3- 3.706e-009 3.440e-009 -8.431 -8.463 -0.032

NaSO4- 3.685e-009 3.420e-009 -8.434 -8.466 -0.032

NaOH 8.449e-012 8.459e-012 -11.073 -11.073 0.000

O(0) 5.076e-004

O2 2.538e-004 2.541e-004 -3.595 -3.595 0.000

S(6) 1.154e-004

SO4-2 9.731e-005 7.261e-005 -4.012 -4.139 -0.127

CaSO4 1.142e-005 1.143e-005 -4.942 -4.942 0.000

MgSO4 6.630e-006 6.637e-006 -5.178 -5.178 0.000

NaSO4- 3.685e-009 3.420e-009 -8.434 -8.466 -0.032

KSO4- 1.757e-009 1.631e-009 -8.755 -8.788 -0.032

HSO4- 5.770e-011 5.356e-011 -10.239 -10.271 -0.032

CaHSO4+ 5.369e-013 4.984e-013 -12.270 -12.302 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.49 -7.86 -8.35 CaCO3

Calcite 0.63 -7.86 -8.49 CaCO3

CO2(g) -2.88 -4.37 -1.49 CO2

Dolomite 1.10 -16.04 -17.14 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.28 -27.44 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.69 -3.60 -2.91 O2

Initial solution 71. 30/8/2012 05:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.045e-004 5.045e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.160

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 314

Density (g/cm3) = 0.99670

Activity of water = 1.000

Ionic strength = 4.781e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.992e-003

Total CO2 (mol/kg) = 2.992e-003

Temperature (deg C) = 27.100

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551612e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.2878 0.7320

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.826e-006 1.693e-006 -5.739 -5.771 -0.033

H+ 7.402e-009 6.918e-009 -8.131 -8.160 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.992e-003

HCO3- 2.853e-003 2.653e-003 -2.545 -2.576 -0.031

CO2 4.022e-005 4.027e-005 -4.396 -4.395 0.000

CaHCO3+ 2.902e-005 2.699e-005 -4.537 -4.569 -0.031

CaCO3 2.540e-005 2.543e-005 -4.595 -4.595 0.000

CO3-2 2.504e-005 1.874e-005 -4.601 -4.727 -0.126

MgHCO3+ 1.247e-005 1.158e-005 -4.904 -4.936 -0.032

MgCO3 6.815e-006 6.822e-006 -5.167 -5.166 0.000

NaHCO3 1.382e-008 1.384e-008 -7.859 -7.859 0.000

NaCO3- 3.874e-009 3.596e-009 -8.412 -8.444 -0.032

Ca 1.100e-003

Ca+2 1.034e-003 7.733e-004 -2.985 -3.112 -0.126

CaHCO3+ 2.902e-005 2.699e-005 -4.537 -4.569 -0.031

CaCO3 2.540e-005 2.543e-005 -4.595 -4.595 0.000

CaSO4 1.141e-005 1.143e-005 -4.943 -4.942 0.000

CaOH+ 1.998e-008 1.855e-008 -7.699 -7.732 -0.032

CaHSO4+ 5.124e-013 4.756e-013 -12.290 -12.323 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 6.630e-028

H2 3.315e-028 3.319e-028 -27.479 -27.479 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.758e-009 1.631e-009 -8.755 -8.787 -0.032

KOH 1.543e-012 1.545e-012 -11.812 -11.811 0.000

Mg 5.184e-004

Mg+2 4.922e-004 3.694e-004 -3.308 -3.433 -0.125

MgHCO3+ 1.247e-005 1.158e-005 -4.904 -4.936 -0.032

MgCO3 6.815e-006 6.822e-006 -5.167 -5.166 0.000

MgSO4 6.628e-006 6.635e-006 -5.179 -5.178 0.000

MgOH+ 2.521e-007 2.340e-007 -6.598 -6.631 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.382e-008 1.384e-008 -7.859 -7.859 0.000

NaCO3- 3.874e-009 3.596e-009 -8.412 -8.444 -0.032

NaSO4- 3.685e-009 3.421e-009 -8.434 -8.466 -0.032

NaOH 8.848e-012 8.857e-012 -11.053 -11.053 0.000

O(0) 5.045e-004

O2 2.523e-004 2.525e-004 -3.598 -3.598 0.000

S(6) 1.154e-004

SO4-2 9.732e-005 7.262e-005 -4.012 -4.139 -0.127

CaSO4 1.141e-005 1.143e-005 -4.943 -4.942 0.000

MgSO4 6.628e-006 6.635e-006 -5.179 -5.178 0.000

NaSO4- 3.685e-009 3.421e-009 -8.434 -8.466 -0.032

KSO4- 1.758e-009 1.631e-009 -8.755 -8.787 -0.032

HSO4- 5.511e-011 5.116e-011 -10.259 -10.291 -0.032

CaHSO4+ 5.124e-013 4.756e-013 -12.290 -12.323 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.51 -7.84 -8.35 CaCO3

Calcite 0.65 -7.84 -8.49 CaCO3

CO2(g) -2.90 -4.40 -1.49 CO2

Dolomite 1.14 -16.00 -17.14 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.32 -27.48 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.69 -3.60 -2.91 O2

Initial solution 72. 30/8/2012 05:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.133e-004 5.133e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.160

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 313

Density (g/cm3) = 0.99673

Activity of water = 1.000

Ionic strength = 4.781e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.992e-003

Total CO2 (mol/kg) = 2.992e-003

Temperature (deg C) = 27.000

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551613e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.2979 0.7324

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.812e-006 1.681e-006 -5.742 -5.775 -0.033

H+ 7.402e-009 6.918e-009 -8.131 -8.160 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.992e-003

HCO3- 2.853e-003 2.653e-003 -2.545 -2.576 -0.031

CO2 4.027e-005 4.032e-005 -4.395 -4.394 0.000

CaHCO3+ 2.899e-005 2.696e-005 -4.538 -4.569 -0.031

CaCO3 2.531e-005 2.534e-005 -4.597 -4.596 0.000

CO3-2 2.500e-005 1.871e-005 -4.602 -4.728 -0.126

MgHCO3+ 1.247e-005 1.158e-005 -4.904 -4.936 -0.032

MgCO3 6.793e-006 6.800e-006 -5.168 -5.167 0.000

NaHCO3 1.383e-008 1.384e-008 -7.859 -7.859 0.000

NaCO3- 3.848e-009 3.572e-009 -8.415 -8.447 -0.032

Ca 1.100e-003

Ca+2 1.034e-003 7.734e-004 -2.985 -3.112 -0.126

CaHCO3+ 2.899e-005 2.696e-005 -4.538 -4.569 -0.031

CaCO3 2.531e-005 2.534e-005 -4.597 -4.596 0.000

CaSO4 1.141e-005 1.142e-005 -4.943 -4.942 0.000

CaOH+ 1.999e-008 1.855e-008 -7.699 -7.732 -0.032

CaHSO4+ 5.115e-013 4.748e-013 -12.291 -12.324 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 6.637e-028

H2 3.318e-028 3.322e-028 -27.479 -27.479 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.755e-009 1.629e-009 -8.756 -8.788 -0.032

KOH 1.543e-012 1.545e-012 -11.812 -11.811 0.000

Mg 5.184e-004

Mg+2 4.923e-004 3.694e-004 -3.308 -3.432 -0.125

MgHCO3+ 1.247e-005 1.158e-005 -4.904 -4.936 -0.032

MgCO3 6.793e-006 6.800e-006 -5.168 -5.167 0.000

MgSO4 6.614e-006 6.621e-006 -5.180 -5.179 0.000

MgOH+ 2.499e-007 2.319e-007 -6.602 -6.635 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.383e-008 1.384e-008 -7.859 -7.859 0.000

NaCO3- 3.848e-009 3.572e-009 -8.415 -8.447 -0.032

NaSO4- 3.684e-009 3.420e-009 -8.434 -8.466 -0.032

NaOH 8.848e-012 8.857e-012 -11.053 -11.053 0.000

O(0) 5.133e-004

O2 2.566e-004 2.569e-004 -3.591 -3.590 0.000

S(6) 1.154e-004

SO4-2 9.734e-005 7.264e-005 -4.012 -4.139 -0.127

CaSO4 1.141e-005 1.142e-005 -4.943 -4.942 0.000

MgSO4 6.614e-006 6.621e-006 -5.180 -5.179 0.000

NaSO4- 3.684e-009 3.420e-009 -8.434 -8.466 -0.032

KSO4- 1.755e-009 1.629e-009 -8.756 -8.788 -0.032

HSO4- 5.500e-011 5.106e-011 -10.260 -10.292 -0.032

CaHSO4+ 5.115e-013 4.748e-013 -12.291 -12.324 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.51 -7.84 -8.35 CaCO3

Calcite 0.65 -7.84 -8.49 CaCO3

CO2(g) -2.90 -4.39 -1.49 CO2

Dolomite 1.14 -16.00 -17.14 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.32 -27.48 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.68 -3.59 -2.91 O2

Initial solution 73. 30/8/2012 05:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.021e-003 3.021e-003

Ca 1.104e-003 1.104e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.933e-004 4.933e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.150

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 314

Density (g/cm3) = 0.99673

Activity of water = 1.000

Ionic strength = 4.794e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.004e-003

Total CO2 (mol/kg) = 3.004e-003

Temperature (deg C) = 27.000

Electrical balance (eq) = -5.188e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.83

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551615e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3036 0.7327

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.771e-006 1.642e-006 -5.752 -5.785 -0.033

H+ 7.575e-009 7.079e-009 -8.121 -8.150 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.004e-003

HCO3- 2.865e-003 2.665e-003 -2.543 -2.574 -0.032

CO2 4.138e-005 4.143e-005 -4.383 -4.383 0.000

CaHCO3+ 2.921e-005 2.717e-005 -4.534 -4.566 -0.032

CaCO3 2.492e-005 2.495e-005 -4.603 -4.603 0.000

CO3-2 2.454e-005 1.836e-005 -4.610 -4.736 -0.126

MgHCO3+ 1.252e-005 1.162e-005 -4.902 -4.935 -0.032

MgCO3 6.665e-006 6.672e-006 -5.176 -5.176 0.000

NaHCO3 1.388e-008 1.390e-008 -7.858 -7.857 0.000

NaCO3- 3.776e-009 3.505e-009 -8.423 -8.455 -0.032

Ca 1.104e-003

Ca+2 1.038e-003 7.761e-004 -2.984 -3.110 -0.126

CaHCO3+ 2.921e-005 2.717e-005 -4.534 -4.566 -0.032

CaCO3 2.492e-005 2.495e-005 -4.603 -4.603 0.000

CaSO4 1.144e-005 1.145e-005 -4.942 -4.941 0.000

CaOH+ 1.960e-008 1.819e-008 -7.708 -7.740 -0.032

CaHSO4+ 5.249e-013 4.872e-013 -12.280 -12.312 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 6.950e-028

H2 3.475e-028 3.479e-028 -27.459 -27.459 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.754e-009 1.628e-009 -8.756 -8.788 -0.032

KOH 1.508e-012 1.510e-012 -11.822 -11.821 0.000

Mg 5.184e-004

Mg+2 4.924e-004 3.694e-004 -3.308 -3.433 -0.125

MgHCO3+ 1.252e-005 1.162e-005 -4.902 -4.935 -0.032

MgCO3 6.665e-006 6.672e-006 -5.176 -5.176 0.000

MgSO4 6.608e-006 6.616e-006 -5.180 -5.179 0.000

MgOH+ 2.442e-007 2.266e-007 -6.612 -6.645 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.388e-008 1.390e-008 -7.858 -7.857 0.000

NaCO3- 3.776e-009 3.505e-009 -8.423 -8.455 -0.032

NaSO4- 3.682e-009 3.417e-009 -8.434 -8.466 -0.032

NaOH 8.645e-012 8.655e-012 -11.063 -11.063 0.000

O(0) 4.933e-004

O2 2.466e-004 2.469e-004 -3.608 -3.607 0.000

S(6) 1.154e-004

SO4-2 9.732e-005 7.260e-005 -4.012 -4.139 -0.127

CaSO4 1.144e-005 1.145e-005 -4.942 -4.941 0.000

MgSO4 6.608e-006 6.616e-006 -5.180 -5.179 0.000

NaSO4- 3.682e-009 3.417e-009 -8.434 -8.466 -0.032

KSO4- 1.754e-009 1.628e-009 -8.756 -8.788 -0.032

HSO4- 5.625e-011 5.221e-011 -10.250 -10.282 -0.032

CaHSO4+ 5.249e-013 4.872e-013 -12.280 -12.312 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.50 -7.85 -8.35 CaCO3

Calcite 0.65 -7.85 -8.49 CaCO3

CO2(g) -2.89 -4.38 -1.49 CO2

Dolomite 1.12 -16.01 -17.14 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.30 -27.46 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.70 -3.61 -2.91 O2

Initial solution 74. 30/8/2012 06:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.021e-003 3.021e-003

Ca 1.104e-003 1.104e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.989e-004 4.989e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.140

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 314

Density (g/cm3) = 0.99673

Activity of water = 1.000

Ionic strength = 4.796e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.007e-003

Total CO2 (mol/kg) = 3.007e-003

Temperature (deg C) = 27.000

Electrical balance (eq) = -5.188e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.83

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551616e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3148 0.7334

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.731e-006 1.605e-006 -5.762 -5.795 -0.033

H+ 7.751e-009 7.244e-009 -8.111 -8.140 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.007e-003

HCO3- 2.868e-003 2.667e-003 -2.542 -2.574 -0.032

CO2 4.238e-005 4.243e-005 -4.373 -4.372 0.000

CaHCO3+ 2.925e-005 2.720e-005 -4.534 -4.565 -0.032

CaCO3 2.439e-005 2.441e-005 -4.613 -4.612 0.000

CO3-2 2.400e-005 1.796e-005 -4.620 -4.746 -0.126

MgHCO3+ 1.254e-005 1.164e-005 -4.902 -4.934 -0.032

MgCO3 6.520e-006 6.527e-006 -5.186 -5.185 0.000

NaHCO3 1.389e-008 1.391e-008 -7.857 -7.857 0.000

NaCO3- 3.693e-009 3.428e-009 -8.433 -8.465 -0.032

Ca 1.104e-003

Ca+2 1.038e-003 7.764e-004 -2.984 -3.110 -0.126

CaHCO3+ 2.925e-005 2.720e-005 -4.534 -4.565 -0.032

CaCO3 2.439e-005 2.441e-005 -4.613 -4.612 0.000

CaSO4 1.144e-005 1.146e-005 -4.941 -4.941 0.000

CaOH+ 1.916e-008 1.779e-008 -7.718 -7.750 -0.032

CaHSO4+ 5.373e-013 4.987e-013 -12.270 -12.302 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 7.277e-028

H2 3.639e-028 3.643e-028 -27.439 -27.439 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.754e-009 1.628e-009 -8.756 -8.788 -0.032

KOH 1.474e-012 1.475e-012 -11.832 -11.831 0.000

Mg 5.184e-004

Mg+2 4.925e-004 3.694e-004 -3.308 -3.432 -0.125

MgHCO3+ 1.254e-005 1.164e-005 -4.902 -4.934 -0.032

MgSO4 6.609e-006 6.617e-006 -5.180 -5.179 0.000

MgCO3 6.520e-006 6.527e-006 -5.186 -5.185 0.000

MgOH+ 2.387e-007 2.215e-007 -6.622 -6.655 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.389e-008 1.391e-008 -7.857 -7.857 0.000

NaCO3- 3.693e-009 3.428e-009 -8.433 -8.465 -0.032

NaSO4- 3.681e-009 3.417e-009 -8.434 -8.466 -0.032

NaOH 8.449e-012 8.458e-012 -11.073 -11.073 0.000

O(0) 4.989e-004

O2 2.494e-004 2.497e-004 -3.603 -3.603 0.000

S(6) 1.154e-004

SO4-2 9.731e-005 7.259e-005 -4.012 -4.139 -0.127

CaSO4 1.144e-005 1.146e-005 -4.941 -4.941 0.000

MgSO4 6.609e-006 6.617e-006 -5.180 -5.179 0.000

NaSO4- 3.681e-009 3.417e-009 -8.434 -8.466 -0.032

KSO4- 1.754e-009 1.628e-009 -8.756 -8.788 -0.032

HSO4- 5.756e-011 5.343e-011 -10.240 -10.272 -0.032

CaHSO4+ 5.373e-013 4.987e-013 -12.270 -12.302 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.49 -7.86 -8.35 CaCO3

Calcite 0.64 -7.86 -8.49 CaCO3

CO2(g) -2.88 -4.37 -1.49 CO2

Dolomite 1.10 -16.03 -17.14 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.28 -27.44 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.70 -3.60 -2.91 O2

Initial solution 75. 30/8/2012 06:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.021e-003 3.021e-003

Ca 1.104e-003 1.104e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.970e-004 4.970e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.150

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 313

Density (g/cm3) = 0.99675

Activity of water = 1.000

Ionic strength = 4.795e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.005e-003

Total CO2 (mol/kg) = 3.005e-003

Temperature (deg C) = 26.900

Electrical balance (eq) = -5.188e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.83

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551615e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3126 0.7330

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.758e-006 1.630e-006 -5.755 -5.788 -0.033

H+ 7.575e-009 7.079e-009 -8.121 -8.150 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.005e-003

HCO3- 2.865e-003 2.665e-003 -2.543 -2.574 -0.032

CO2 4.144e-005 4.148e-005 -4.383 -4.382 0.000

CaHCO3+ 2.918e-005 2.714e-005 -4.535 -4.566 -0.032

CaCO3 2.483e-005 2.486e-005 -4.605 -4.605 0.000

CO3-2 2.450e-005 1.833e-005 -4.611 -4.737 -0.126

MgHCO3+ 1.252e-005 1.162e-005 -4.902 -4.935 -0.032

MgCO3 6.644e-006 6.651e-006 -5.178 -5.177 0.000

NaHCO3 1.388e-008 1.390e-008 -7.857 -7.857 0.000

NaCO3- 3.750e-009 3.481e-009 -8.426 -8.458 -0.032

Ca 1.104e-003

Ca+2 1.038e-003 7.762e-004 -2.984 -3.110 -0.126

CaHCO3+ 2.918e-005 2.714e-005 -4.535 -4.566 -0.032

CaCO3 2.483e-005 2.486e-005 -4.605 -4.605 0.000

CaSO4 1.143e-005 1.145e-005 -4.942 -4.941 0.000

CaOH+ 1.960e-008 1.819e-008 -7.708 -7.740 -0.032

CaHSO4+ 5.239e-013 4.863e-013 -12.281 -12.313 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 6.956e-028

H2 3.478e-028 3.482e-028 -27.459 -27.458 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.751e-009 1.626e-009 -8.757 -8.789 -0.032

KOH 1.508e-012 1.510e-012 -11.822 -11.821 0.000

Mg 5.184e-004

Mg+2 4.924e-004 3.694e-004 -3.308 -3.433 -0.125

MgHCO3+ 1.252e-005 1.162e-005 -4.902 -4.935 -0.032

MgCO3 6.644e-006 6.651e-006 -5.178 -5.177 0.000

MgSO4 6.594e-006 6.601e-006 -5.181 -5.180 0.000

MgOH+ 2.420e-007 2.246e-007 -6.616 -6.649 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.388e-008 1.390e-008 -7.857 -7.857 0.000

NaCO3- 3.750e-009 3.481e-009 -8.426 -8.458 -0.032

NaSO4- 3.680e-009 3.416e-009 -8.434 -8.466 -0.032

NaOH 8.646e-012 8.655e-012 -11.063 -11.063 0.000

O(0) 4.970e-004

O2 2.485e-004 2.488e-004 -3.605 -3.604 0.000

S(6) 1.154e-004

SO4-2 9.734e-005 7.261e-005 -4.012 -4.139 -0.127

CaSO4 1.143e-005 1.145e-005 -4.942 -4.941 0.000

MgSO4 6.594e-006 6.601e-006 -5.181 -5.180 0.000

NaSO4- 3.680e-009 3.416e-009 -8.434 -8.466 -0.032

KSO4- 1.751e-009 1.626e-009 -8.757 -8.789 -0.032

HSO4- 5.614e-011 5.211e-011 -10.251 -10.283 -0.032

CaHSO4+ 5.239e-013 4.863e-013 -12.281 -12.313 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.50 -7.85 -8.35 CaCO3

Calcite 0.64 -7.85 -8.49 CaCO3

CO2(g) -2.89 -4.38 -1.49 CO2

Dolomite 1.12 -16.02 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.30 -27.46 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.70 -3.60 -2.91 O2

Initial solution 76. 30/8/2012 06:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.021e-003 3.021e-003

Ca 1.104e-003 1.104e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.995e-004 4.995e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.150

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 313

Density (g/cm3) = 0.99675

Activity of water = 1.000

Ionic strength = 4.795e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.005e-003

Total CO2 (mol/kg) = 3.005e-003

Temperature (deg C) = 26.900

Electrical balance (eq) = -5.188e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.83

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551615e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3131 0.7330

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.758e-006 1.630e-006 -5.755 -5.788 -0.033

H+ 7.575e-009 7.079e-009 -8.121 -8.150 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.005e-003

HCO3- 2.865e-003 2.665e-003 -2.543 -2.574 -0.032

CO2 4.144e-005 4.148e-005 -4.383 -4.382 0.000

CaHCO3+ 2.918e-005 2.714e-005 -4.535 -4.566 -0.032

CaCO3 2.483e-005 2.486e-005 -4.605 -4.605 0.000

CO3-2 2.450e-005 1.833e-005 -4.611 -4.737 -0.126

MgHCO3+ 1.252e-005 1.162e-005 -4.902 -4.935 -0.032

MgCO3 6.644e-006 6.651e-006 -5.178 -5.177 0.000

NaHCO3 1.388e-008 1.390e-008 -7.857 -7.857 0.000

NaCO3- 3.750e-009 3.481e-009 -8.426 -8.458 -0.032

Ca 1.104e-003

Ca+2 1.038e-003 7.762e-004 -2.984 -3.110 -0.126

CaHCO3+ 2.918e-005 2.714e-005 -4.535 -4.566 -0.032

CaCO3 2.483e-005 2.486e-005 -4.605 -4.605 0.000

CaSO4 1.143e-005 1.145e-005 -4.942 -4.941 0.000

CaOH+ 1.960e-008 1.819e-008 -7.708 -7.740 -0.032

CaHSO4+ 5.239e-013 4.863e-013 -12.281 -12.313 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 6.956e-028

H2 3.478e-028 3.482e-028 -27.459 -27.458 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.751e-009 1.626e-009 -8.757 -8.789 -0.032

KOH 1.508e-012 1.510e-012 -11.822 -11.821 0.000

Mg 5.184e-004

Mg+2 4.924e-004 3.694e-004 -3.308 -3.433 -0.125

MgHCO3+ 1.252e-005 1.162e-005 -4.902 -4.935 -0.032

MgCO3 6.644e-006 6.651e-006 -5.178 -5.177 0.000

MgSO4 6.594e-006 6.601e-006 -5.181 -5.180 0.000

MgOH+ 2.420e-007 2.246e-007 -6.616 -6.649 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.388e-008 1.390e-008 -7.857 -7.857 0.000

NaCO3- 3.750e-009 3.481e-009 -8.426 -8.458 -0.032

NaSO4- 3.680e-009 3.416e-009 -8.434 -8.466 -0.032

NaOH 8.646e-012 8.655e-012 -11.063 -11.063 0.000

O(0) 4.995e-004

O2 2.498e-004 2.500e-004 -3.602 -3.602 0.000

S(6) 1.154e-004

SO4-2 9.734e-005 7.261e-005 -4.012 -4.139 -0.127

CaSO4 1.143e-005 1.145e-005 -4.942 -4.941 0.000

MgSO4 6.594e-006 6.601e-006 -5.181 -5.180 0.000

NaSO4- 3.680e-009 3.416e-009 -8.434 -8.466 -0.032

KSO4- 1.751e-009 1.626e-009 -8.757 -8.789 -0.032

HSO4- 5.614e-011 5.211e-011 -10.251 -10.283 -0.032

CaHSO4+ 5.239e-013 4.863e-013 -12.281 -12.313 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.50 -7.85 -8.35 CaCO3

Calcite 0.64 -7.85 -8.49 CaCO3

CO2(g) -2.89 -4.38 -1.49 CO2

Dolomite 1.12 -16.02 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.30 -27.46 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.70 -3.60 -2.91 O2

Initial solution 77. 30/8/2012 06:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.926e-004 4.926e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.140

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 312

Density (g/cm3) = 0.99678

Activity of water = 1.000

Ionic strength = 4.785e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.997e-003

Total CO2 (mol/kg) = 2.997e-003

Temperature (deg C) = 26.800

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551612e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3298 0.7338

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.705e-006 1.581e-006 -5.768 -5.801 -0.033

H+ 7.751e-009 7.244e-009 -8.111 -8.140 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.997e-003

HCO3- 2.859e-003 2.659e-003 -2.544 -2.575 -0.031

CO2 4.235e-005 4.240e-005 -4.373 -4.373 0.000

CaHCO3+ 2.900e-005 2.697e-005 -4.538 -4.569 -0.031

CaCO3 2.405e-005 2.408e-005 -4.619 -4.618 0.000

CO3-2 2.383e-005 1.783e-005 -4.623 -4.749 -0.126

MgHCO3+ 1.249e-005 1.160e-005 -4.903 -4.936 -0.032

MgCO3 6.460e-006 6.467e-006 -5.190 -5.189 0.000

NaHCO3 1.385e-008 1.387e-008 -7.858 -7.858 0.000

NaCO3- 3.631e-009 3.371e-009 -8.440 -8.472 -0.032

Ca 1.100e-003

Ca+2 1.035e-003 7.744e-004 -2.985 -3.111 -0.126

CaHCO3+ 2.900e-005 2.697e-005 -4.538 -4.569 -0.031

CaCO3 2.405e-005 2.408e-005 -4.619 -4.618 0.000

CaSO4 1.140e-005 1.142e-005 -4.943 -4.942 0.000

CaOH+ 1.911e-008 1.774e-008 -7.719 -7.751 -0.032

CaHSO4+ 5.340e-013 4.957e-013 -12.272 -12.305 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 7.291e-028

H2 3.646e-028 3.650e-028 -27.438 -27.438 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.749e-009 1.624e-009 -8.757 -8.789 -0.032

KOH 1.474e-012 1.475e-012 -11.832 -11.831 0.000

Mg 5.184e-004

Mg+2 4.926e-004 3.697e-004 -3.307 -3.432 -0.125

MgHCO3+ 1.249e-005 1.160e-005 -4.903 -4.936 -0.032

MgSO4 6.587e-006 6.594e-006 -5.181 -5.181 0.000

MgCO3 6.460e-006 6.467e-006 -5.190 -5.189 0.000

MgOH+ 2.346e-007 2.177e-007 -6.630 -6.662 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.385e-008 1.387e-008 -7.858 -7.858 0.000

NaSO4- 3.681e-009 3.417e-009 -8.434 -8.466 -0.032

NaCO3- 3.631e-009 3.371e-009 -8.440 -8.472 -0.032

NaOH 8.450e-012 8.459e-012 -11.073 -11.073 0.000

O(0) 4.926e-004

O2 2.463e-004 2.466e-004 -3.609 -3.608 0.000

S(6) 1.154e-004

SO4-2 9.737e-005 7.266e-005 -4.012 -4.139 -0.127

CaSO4 1.140e-005 1.142e-005 -4.943 -4.942 0.000

MgSO4 6.587e-006 6.594e-006 -5.181 -5.181 0.000

NaSO4- 3.681e-009 3.417e-009 -8.434 -8.466 -0.032

KSO4- 1.749e-009 1.624e-009 -8.757 -8.789 -0.032

HSO4- 5.736e-011 5.324e-011 -10.241 -10.274 -0.032

CaHSO4+ 5.340e-013 4.957e-013 -12.272 -12.305 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.49 -7.86 -8.35 CaCO3

Calcite 0.63 -7.86 -8.49 CaCO3

CO2(g) -2.88 -4.37 -1.49 CO2

Dolomite 1.09 -16.04 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.28 -27.44 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.70 -3.61 -2.91 O2

Initial solution 78. 30/8/2012 07:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.021e-003 3.021e-003

Ca 1.104e-003 1.104e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.920e-004 4.920e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.140

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 313

Density (g/cm3) = 0.99678

Activity of water = 1.000

Ionic strength = 4.796e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.007e-003

Total CO2 (mol/kg) = 3.007e-003

Temperature (deg C) = 26.800

Electrical balance (eq) = -5.188e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.83

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551615e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3296 0.7338

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.705e-006 1.581e-006 -5.768 -5.801 -0.033

H+ 7.751e-009 7.244e-009 -8.111 -8.140 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.007e-003

HCO3- 2.868e-003 2.668e-003 -2.542 -2.574 -0.032

CO2 4.249e-005 4.254e-005 -4.372 -4.371 0.000

CaHCO3+ 2.918e-005 2.714e-005 -4.535 -4.566 -0.032

CaCO3 2.420e-005 2.423e-005 -4.616 -4.616 0.000

CO3-2 2.392e-005 1.789e-005 -4.621 -4.747 -0.126

MgHCO3+ 1.253e-005 1.163e-005 -4.902 -4.934 -0.032

MgCO3 6.479e-006 6.486e-006 -5.189 -5.188 0.000

NaHCO3 1.390e-008 1.391e-008 -7.857 -7.857 0.000

NaCO3- 3.643e-009 3.382e-009 -8.438 -8.471 -0.032

Ca 1.104e-003

Ca+2 1.039e-003 7.767e-004 -2.983 -3.110 -0.126

CaHCO3+ 2.918e-005 2.714e-005 -4.535 -4.566 -0.032

CaCO3 2.420e-005 2.423e-005 -4.616 -4.616 0.000

CaSO4 1.143e-005 1.144e-005 -4.942 -4.941 0.000

CaOH+ 1.917e-008 1.779e-008 -7.717 -7.750 -0.032

CaHSO4+ 5.353e-013 4.969e-013 -12.271 -12.304 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 7.291e-028

H2 3.646e-028 3.650e-028 -27.438 -27.438 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.748e-009 1.623e-009 -8.757 -8.790 -0.032

KOH 1.474e-012 1.475e-012 -11.832 -11.831 0.000

Mg 5.184e-004

Mg+2 4.926e-004 3.695e-004 -3.308 -3.432 -0.125

MgHCO3+ 1.253e-005 1.163e-005 -4.902 -4.934 -0.032

MgSO4 6.581e-006 6.588e-006 -5.182 -5.181 0.000

MgCO3 6.479e-006 6.486e-006 -5.189 -5.188 0.000

MgOH+ 2.345e-007 2.177e-007 -6.630 -6.662 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.390e-008 1.391e-008 -7.857 -7.857 0.000

NaSO4- 3.679e-009 3.415e-009 -8.434 -8.467 -0.032

NaCO3- 3.643e-009 3.382e-009 -8.438 -8.471 -0.032

NaOH 8.449e-012 8.458e-012 -11.073 -11.073 0.000

O(0) 4.920e-004

O2 2.460e-004 2.463e-004 -3.609 -3.609 0.000

S(6) 1.154e-004

SO4-2 9.735e-005 7.263e-005 -4.012 -4.139 -0.127

CaSO4 1.143e-005 1.144e-005 -4.942 -4.941 0.000

MgSO4 6.581e-006 6.588e-006 -5.182 -5.181 0.000

NaSO4- 3.679e-009 3.415e-009 -8.434 -8.467 -0.032

KSO4- 1.748e-009 1.623e-009 -8.757 -8.790 -0.032

HSO4- 5.733e-011 5.322e-011 -10.242 -10.274 -0.032

CaHSO4+ 5.353e-013 4.969e-013 -12.271 -12.304 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.49 -7.86 -8.35 CaCO3

Calcite 0.63 -7.86 -8.49 CaCO3

CO2(g) -2.88 -4.37 -1.49 CO2

Dolomite 1.09 -16.04 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.28 -27.44 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.70 -3.61 -2.91 O2

Initial solution 79. 30/8/2012 07:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.021e-003 3.021e-003

Ca 1.104e-003 1.104e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.908e-004 4.908e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.150

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 312

Density (g/cm3) = 0.99681

Activity of water = 1.000

Ionic strength = 4.796e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.005e-003

Total CO2 (mol/kg) = 3.005e-003

Temperature (deg C) = 26.700

Electrical balance (eq) = -5.188e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.83

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551614e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3276 0.7334

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.732e-006 1.606e-006 -5.761 -5.794 -0.033

H+ 7.575e-009 7.079e-009 -8.121 -8.150 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.005e-003

HCO3- 2.866e-003 2.666e-003 -2.543 -2.574 -0.032

CO2 4.154e-005 4.159e-005 -4.382 -4.381 0.000

CaHCO3+ 2.911e-005 2.708e-005 -4.536 -4.567 -0.032

CaCO3 2.464e-005 2.467e-005 -4.608 -4.608 0.000

CO3-2 2.441e-005 1.826e-005 -4.612 -4.738 -0.126

MgHCO3+ 1.251e-005 1.162e-005 -4.903 -4.935 -0.032

MgCO3 6.601e-006 6.609e-006 -5.180 -5.180 0.000

NaHCO3 1.389e-008 1.390e-008 -7.857 -7.857 0.000

NaCO3- 3.700e-009 3.434e-009 -8.432 -8.464 -0.032

Ca 1.104e-003

Ca+2 1.038e-003 7.765e-004 -2.984 -3.110 -0.126

CaHCO3+ 2.911e-005 2.708e-005 -4.536 -4.567 -0.032

CaCO3 2.464e-005 2.467e-005 -4.608 -4.608 0.000

CaSO4 1.142e-005 1.143e-005 -4.942 -4.942 0.000

CaOH+ 1.961e-008 1.820e-008 -7.708 -7.740 -0.032

CaHSO4+ 5.220e-013 4.846e-013 -12.282 -12.315 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 6.970e-028

H2 3.485e-028 3.489e-028 -27.458 -27.457 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.746e-009 1.621e-009 -8.758 -8.790 -0.032

KOH 1.508e-012 1.510e-012 -11.822 -11.821 0.000

Mg 5.184e-004

Mg+2 4.925e-004 3.695e-004 -3.308 -3.432 -0.125

MgHCO3+ 1.251e-005 1.162e-005 -4.903 -4.935 -0.032

MgCO3 6.601e-006 6.609e-006 -5.180 -5.180 0.000

MgSO4 6.565e-006 6.573e-006 -5.183 -5.182 0.000

MgOH+ 2.378e-007 2.207e-007 -6.624 -6.656 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.389e-008 1.390e-008 -7.857 -7.857 0.000

NaCO3- 3.700e-009 3.434e-009 -8.432 -8.464 -0.032

NaSO4- 3.678e-009 3.414e-009 -8.434 -8.467 -0.032

NaOH 8.646e-012 8.655e-012 -11.063 -11.063 0.000

O(0) 4.908e-004

O2 2.454e-004 2.456e-004 -3.610 -3.610 0.000

S(6) 1.154e-004

SO4-2 9.738e-005 7.265e-005 -4.012 -4.139 -0.127

CaSO4 1.142e-005 1.143e-005 -4.942 -4.942 0.000

MgSO4 6.565e-006 6.573e-006 -5.183 -5.182 0.000

NaSO4- 3.678e-009 3.414e-009 -8.434 -8.467 -0.032

KSO4- 1.746e-009 1.621e-009 -8.758 -8.790 -0.032

HSO4- 5.592e-011 5.191e-011 -10.252 -10.285 -0.032

CaHSO4+ 5.220e-013 4.846e-013 -12.282 -12.315 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.50 -7.85 -8.35 CaCO3

Calcite 0.64 -7.85 -8.49 CaCO3

CO2(g) -2.89 -4.38 -1.49 CO2

Dolomite 1.11 -16.02 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.30 -27.46 -3.16 H2

H2O(g) -1.47 -0.00 1.47 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.71 -3.61 -2.90 O2

Initial solution 80. 30/8/2012 07:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.021e-003 3.021e-003

Ca 1.104e-003 1.104e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.195e-004 5.195e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.150

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 312

Density (g/cm3) = 0.99681

Activity of water = 1.000

Ionic strength = 4.796e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.005e-003

Total CO2 (mol/kg) = 3.005e-003

Temperature (deg C) = 26.700

Electrical balance (eq) = -5.188e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.83

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551617e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3337 0.7338

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.732e-006 1.606e-006 -5.761 -5.794 -0.033

H+ 7.575e-009 7.079e-009 -8.121 -8.150 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.005e-003

HCO3- 2.866e-003 2.666e-003 -2.543 -2.574 -0.032

CO2 4.154e-005 4.159e-005 -4.382 -4.381 0.000

CaHCO3+ 2.911e-005 2.708e-005 -4.536 -4.567 -0.032

CaCO3 2.464e-005 2.467e-005 -4.608 -4.608 0.000

CO3-2 2.441e-005 1.826e-005 -4.612 -4.738 -0.126

MgHCO3+ 1.251e-005 1.162e-005 -4.903 -4.935 -0.032

MgCO3 6.601e-006 6.609e-006 -5.180 -5.180 0.000

NaHCO3 1.389e-008 1.390e-008 -7.857 -7.857 0.000

NaCO3- 3.700e-009 3.434e-009 -8.432 -8.464 -0.032

Ca 1.104e-003

Ca+2 1.038e-003 7.765e-004 -2.984 -3.110 -0.126

CaHCO3+ 2.911e-005 2.708e-005 -4.536 -4.567 -0.032

CaCO3 2.464e-005 2.467e-005 -4.608 -4.608 0.000

CaSO4 1.142e-005 1.143e-005 -4.942 -4.942 0.000

CaOH+ 1.961e-008 1.820e-008 -7.708 -7.740 -0.032

CaHSO4+ 5.220e-013 4.846e-013 -12.282 -12.315 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 6.970e-028

H2 3.485e-028 3.489e-028 -27.458 -27.457 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.746e-009 1.621e-009 -8.758 -8.790 -0.032

KOH 1.508e-012 1.510e-012 -11.822 -11.821 0.000

Mg 5.184e-004

Mg+2 4.925e-004 3.695e-004 -3.308 -3.432 -0.125

MgHCO3+ 1.251e-005 1.162e-005 -4.903 -4.935 -0.032

MgCO3 6.601e-006 6.609e-006 -5.180 -5.180 0.000

MgSO4 6.565e-006 6.573e-006 -5.183 -5.182 0.000

MgOH+ 2.378e-007 2.207e-007 -6.624 -6.656 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.389e-008 1.390e-008 -7.857 -7.857 0.000

NaCO3- 3.700e-009 3.434e-009 -8.432 -8.464 -0.032

NaSO4- 3.678e-009 3.414e-009 -8.434 -8.467 -0.032

NaOH 8.646e-012 8.655e-012 -11.063 -11.063 0.000

O(0) 5.195e-004

O2 2.598e-004 2.600e-004 -3.585 -3.585 0.000

S(6) 1.154e-004

SO4-2 9.738e-005 7.265e-005 -4.012 -4.139 -0.127

CaSO4 1.142e-005 1.143e-005 -4.942 -4.942 0.000

MgSO4 6.565e-006 6.573e-006 -5.183 -5.182 0.000

NaSO4- 3.678e-009 3.414e-009 -8.434 -8.467 -0.032

KSO4- 1.746e-009 1.621e-009 -8.758 -8.790 -0.032

HSO4- 5.592e-011 5.191e-011 -10.252 -10.285 -0.032

CaHSO4+ 5.220e-013 4.846e-013 -12.282 -12.315 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.50 -7.85 -8.35 CaCO3

Calcite 0.64 -7.85 -8.49 CaCO3

CO2(g) -2.89 -4.38 -1.49 CO2

Dolomite 1.11 -16.02 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.30 -27.46 -3.16 H2

H2O(g) -1.47 -0.00 1.47 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.68 -3.58 -2.90 O2

Initial solution 81. 30/8/2012 07:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.039e-004 5.039e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.160

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 311

Density (g/cm3) = 0.99681

Activity of water = 1.000

Ionic strength = 4.782e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.992e-003

Total CO2 (mol/kg) = 2.992e-003

Temperature (deg C) = 26.700

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551612e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3204 0.7330

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.772e-006 1.644e-006 -5.751 -5.784 -0.033

H+ 7.402e-009 6.918e-009 -8.131 -8.160 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.992e-003

HCO3- 2.854e-003 2.655e-003 -2.545 -2.576 -0.031

CO2 4.043e-005 4.047e-005 -4.393 -4.393 0.000

CaHCO3+ 2.889e-005 2.687e-005 -4.539 -4.571 -0.031

CaCO3 2.503e-005 2.505e-005 -4.602 -4.601 0.000

CO3-2 2.486e-005 1.861e-005 -4.604 -4.730 -0.126

MgHCO3+ 1.246e-005 1.157e-005 -4.904 -4.937 -0.032

MgCO3 6.728e-006 6.735e-006 -5.172 -5.172 0.000

NaHCO3 1.383e-008 1.385e-008 -7.859 -7.859 0.000

NaCO3- 3.770e-009 3.500e-009 -8.424 -8.456 -0.032

Ca 1.100e-003

Ca+2 1.035e-003 7.738e-004 -2.985 -3.111 -0.126

CaHCO3+ 2.889e-005 2.687e-005 -4.539 -4.571 -0.031

CaCO3 2.503e-005 2.505e-005 -4.602 -4.601 0.000

CaSO4 1.139e-005 1.140e-005 -4.943 -4.943 0.000

CaOH+ 1.999e-008 1.856e-008 -7.699 -7.731 -0.032

CaHSO4+ 5.087e-013 4.722e-013 -12.294 -12.326 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 6.656e-028

H2 3.328e-028 3.332e-028 -27.478 -27.477 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.747e-009 1.622e-009 -8.758 -8.790 -0.032

KOH 1.543e-012 1.545e-012 -11.812 -11.811 0.000

Mg 5.184e-004

Mg+2 4.924e-004 3.695e-004 -3.308 -3.432 -0.125

MgHCO3+ 1.246e-005 1.157e-005 -4.904 -4.937 -0.032

MgCO3 6.728e-006 6.735e-006 -5.172 -5.172 0.000

MgSO4 6.571e-006 6.578e-006 -5.182 -5.182 0.000

MgOH+ 2.434e-007 2.259e-007 -6.614 -6.646 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.383e-008 1.385e-008 -7.859 -7.859 0.000

NaCO3- 3.770e-009 3.500e-009 -8.424 -8.456 -0.032

NaSO4- 3.680e-009 3.416e-009 -8.434 -8.466 -0.032

NaOH 8.848e-012 8.858e-012 -11.053 -11.053 0.000

O(0) 5.039e-004

O2 2.519e-004 2.522e-004 -3.599 -3.598 0.000

S(6) 1.154e-004

SO4-2 9.740e-005 7.270e-005 -4.011 -4.138 -0.127

CaSO4 1.139e-005 1.140e-005 -4.943 -4.943 0.000

MgSO4 6.571e-006 6.578e-006 -5.182 -5.182 0.000

NaSO4- 3.680e-009 3.416e-009 -8.434 -8.466 -0.032

KSO4- 1.747e-009 1.622e-009 -8.758 -8.790 -0.032

HSO4- 5.468e-011 5.076e-011 -10.262 -10.294 -0.032

CaHSO4+ 5.087e-013 4.722e-013 -12.294 -12.326 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.51 -7.84 -8.35 CaCO3

Calcite 0.65 -7.84 -8.49 CaCO3

CO2(g) -2.91 -4.39 -1.49 CO2

Dolomite 1.12 -16.00 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.32 -27.48 -3.16 H2

H2O(g) -1.47 -0.00 1.47 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.69 -3.60 -2.90 O2

Initial solution 82. 30/8/2012 08:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.949e-003 2.949e-003

Ca 1.077e-003 1.077e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.114e-004 5.114e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.160

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 306

Density (g/cm3) = 0.99681

Activity of water = 1.000

Ionic strength = 4.712e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.931e-003

Total CO2 (mol/kg) = 2.931e-003

Temperature (deg C) = 26.700

Electrical balance (eq) = -3.183e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.52

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551595e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3220 0.7331

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.771e-006 1.644e-006 -5.752 -5.784 -0.032

H+ 7.399e-009 6.918e-009 -8.131 -8.160 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.931e-003

HCO3- 2.797e-003 2.602e-003 -2.553 -2.585 -0.031

CO2 3.963e-005 3.968e-005 -4.402 -4.401 0.000

CaHCO3+ 2.781e-005 2.587e-005 -4.556 -4.587 -0.031

CO3-2 2.433e-005 1.824e-005 -4.614 -4.739 -0.125

CaCO3 2.410e-005 2.413e-005 -4.618 -4.618 0.000

MgHCO3+ 1.224e-005 1.137e-005 -4.912 -4.944 -0.032

MgCO3 6.612e-006 6.619e-006 -5.180 -5.179 0.000

NaHCO3 1.357e-008 1.358e-008 -7.868 -7.867 0.000

NaCO3- 3.696e-009 3.433e-009 -8.432 -8.464 -0.032

Ca 1.077e-003

Ca+2 1.014e-003 7.601e-004 -2.994 -3.119 -0.125

CaHCO3+ 2.781e-005 2.587e-005 -4.556 -4.587 -0.031

CaCO3 2.410e-005 2.413e-005 -4.618 -4.618 0.000

CaSO4 1.122e-005 1.124e-005 -4.950 -4.949 0.000

CaOH+ 1.963e-008 1.823e-008 -7.707 -7.739 -0.032

CaHSO4+ 5.010e-013 4.654e-013 -12.300 -12.332 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.274 -0.032

H(0) 6.657e-028

H2 3.328e-028 3.332e-028 -27.478 -27.477 0.000

K 3.325e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.753e-009 1.628e-009 -8.756 -8.788 -0.032

KOH 1.544e-012 1.546e-012 -11.811 -11.811 0.000

Mg 5.184e-004

Mg+2 4.927e-004 3.705e-004 -3.307 -3.431 -0.124

MgHCO3+ 1.224e-005 1.137e-005 -4.912 -4.944 -0.032

MgCO3 6.612e-006 6.619e-006 -5.180 -5.179 0.000

MgSO4 6.608e-006 6.616e-006 -5.180 -5.179 0.000

MgOH+ 2.438e-007 2.265e-007 -6.613 -6.645 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.281e-006 -5.001 -5.032 -0.032

NaHCO3 1.357e-008 1.358e-008 -7.868 -7.867 0.000

NaCO3- 3.696e-009 3.433e-009 -8.432 -8.464 -0.032

NaSO4- 3.692e-009 3.429e-009 -8.433 -8.465 -0.032

NaOH 8.853e-012 8.862e-012 -11.053 -11.052 0.000

O(0) 5.114e-004

O2 2.557e-004 2.560e-004 -3.592 -3.592 0.000

S(6) 1.154e-004

SO4-2 9.753e-005 7.293e-005 -4.011 -4.137 -0.126

CaSO4 1.122e-005 1.124e-005 -4.950 -4.949 0.000

MgSO4 6.608e-006 6.616e-006 -5.180 -5.179 0.000

NaSO4- 3.692e-009 3.429e-009 -8.433 -8.465 -0.032

KSO4- 1.753e-009 1.628e-009 -8.756 -8.788 -0.032

HSO4- 5.483e-011 5.092e-011 -10.261 -10.293 -0.032

CaHSO4+ 5.010e-013 4.654e-013 -12.300 -12.332 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.26 -4.37 CaSO4

Aragonite 0.49 -7.86 -8.35 CaCO3

Calcite 0.63 -7.86 -8.49 CaCO3

CO2(g) -2.91 -4.40 -1.49 CO2

Dolomite 1.10 -16.03 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.32 -27.48 -3.16 H2

H2O(g) -1.47 -0.00 1.47 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.69 -3.59 -2.90 O2

Initial solution 83. 30/8/2012 08:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.283e-004 5.283e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.130

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 311

Density (g/cm3) = 0.99678

Activity of water = 1.000

Ionic strength = 4.774e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.989e-003

Total CO2 (mol/kg) = 2.989e-003

Temperature (deg C) = 26.800

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 7

Total H = 1.110153e+002

Total O = 5.551613e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3474 0.7348

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.666e-006 1.545e-006 -5.778 -5.811 -0.033

H+ 7.931e-009 7.413e-009 -8.101 -8.130 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.989e-003

HCO3- 2.851e-003 2.652e-003 -2.545 -2.576 -0.031

CO2 4.323e-005 4.328e-005 -4.364 -4.364 0.000

CaHCO3+ 2.885e-005 2.684e-005 -4.540 -4.571 -0.031

CaCO3 2.339e-005 2.341e-005 -4.631 -4.631 0.000

CO3-2 2.322e-005 1.738e-005 -4.634 -4.760 -0.126

MgHCO3+ 1.247e-005 1.158e-005 -4.904 -4.936 -0.032

MgCO3 6.301e-006 6.308e-006 -5.201 -5.200 0.000

NaHCO3 1.382e-008 1.384e-008 -7.859 -7.859 0.000

NaCO3- 3.540e-009 3.286e-009 -8.451 -8.483 -0.032

Ca 1.096e-003

Ca+2 1.032e-003 7.724e-004 -2.986 -3.112 -0.126

CaHCO3+ 2.885e-005 2.684e-005 -4.540 -4.571 -0.031

CaCO3 2.339e-005 2.341e-005 -4.631 -4.631 0.000

CaSO4 1.138e-005 1.139e-005 -4.944 -4.943 0.000

CaOH+ 1.863e-008 1.729e-008 -7.730 -7.762 -0.032

CaHSO4+ 5.453e-013 5.062e-013 -12.263 -12.296 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 7.635e-028

H2 3.818e-028 3.822e-028 -27.418 -27.418 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.750e-009 1.625e-009 -8.757 -8.789 -0.032

KOH 1.440e-012 1.442e-012 -11.842 -11.841 0.000

Mg 5.184e-004

Mg+2 4.928e-004 3.699e-004 -3.307 -3.432 -0.125

MgHCO3+ 1.247e-005 1.158e-005 -4.904 -4.936 -0.032

MgSO4 6.594e-006 6.601e-006 -5.181 -5.180 0.000

MgCO3 6.301e-006 6.308e-006 -5.201 -5.200 0.000

MgOH+ 2.294e-007 2.129e-007 -6.639 -6.672 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.382e-008 1.384e-008 -7.859 -7.859 0.000

NaSO4- 3.682e-009 3.418e-009 -8.434 -8.466 -0.032

NaCO3- 3.540e-009 3.286e-009 -8.451 -8.483 -0.032

NaOH 8.258e-012 8.267e-012 -11.083 -11.083 0.000

O(0) 5.283e-004

O2 2.641e-004 2.644e-004 -3.578 -3.578 0.000

S(6) 1.154e-004

SO4-2 9.739e-005 7.270e-005 -4.011 -4.138 -0.127

CaSO4 1.138e-005 1.139e-005 -4.944 -4.943 0.000

MgSO4 6.594e-006 6.601e-006 -5.181 -5.180 0.000

NaSO4- 3.682e-009 3.418e-009 -8.434 -8.466 -0.032

KSO4- 1.750e-009 1.625e-009 -8.757 -8.789 -0.032

HSO4- 5.872e-011 5.451e-011 -10.231 -10.264 -0.032

CaHSO4+ 5.453e-013 5.062e-013 -12.263 -12.296 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.48 -7.87 -8.35 CaCO3

Calcite 0.62 -7.87 -8.49 CaCO3

CO2(g) -2.87 -4.36 -1.49 CO2

Dolomite 1.07 -16.06 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.26 -27.42 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.67 -3.58 -2.91 O2

Initial solution 84. 30/8/2012 08:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.264e-004 5.264e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.150

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 311

Density (g/cm3) = 0.99678

Activity of water = 1.000

Ionic strength = 4.772e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.984e-003

Total CO2 (mol/kg) = 2.984e-003

Temperature (deg C) = 26.800

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551612e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3270 0.7336

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.745e-006 1.618e-006 -5.758 -5.791 -0.033

H+ 7.574e-009 7.079e-009 -8.121 -8.150 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.984e-003

HCO3- 2.847e-003 2.648e-003 -2.546 -2.577 -0.031

CO2 4.122e-005 4.126e-005 -4.385 -4.384 0.000

CaHCO3+ 2.878e-005 2.677e-005 -4.541 -4.572 -0.031

CaCO3 2.443e-005 2.445e-005 -4.612 -4.612 0.000

CO3-2 2.428e-005 1.817e-005 -4.615 -4.741 -0.126

MgHCO3+ 1.244e-005 1.155e-005 -4.905 -4.937 -0.032

MgCO3 6.584e-006 6.591e-006 -5.181 -5.181 0.000

NaHCO3 1.380e-008 1.381e-008 -7.860 -7.860 0.000

NaCO3- 3.701e-009 3.436e-009 -8.432 -8.464 -0.032

Ca 1.096e-003

Ca+2 1.031e-003 7.718e-004 -2.987 -3.113 -0.126

CaHCO3+ 2.878e-005 2.677e-005 -4.541 -4.572 -0.031

CaCO3 2.443e-005 2.445e-005 -4.612 -4.612 0.000

CaSO4 1.137e-005 1.139e-005 -4.944 -4.944 0.000

CaOH+ 1.949e-008 1.809e-008 -7.710 -7.743 -0.032

CaHSO4+ 5.204e-013 4.831e-013 -12.284 -12.316 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 6.963e-028

H2 3.482e-028 3.485e-028 -27.458 -27.458 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.751e-009 1.625e-009 -8.757 -8.789 -0.032

KOH 1.508e-012 1.510e-012 -11.822 -11.821 0.000

Mg 5.184e-004

Mg+2 4.925e-004 3.697e-004 -3.308 -3.432 -0.125

MgHCO3+ 1.244e-005 1.155e-005 -4.905 -4.937 -0.032

MgSO4 6.592e-006 6.599e-006 -5.181 -5.180 0.000

MgCO3 6.584e-006 6.591e-006 -5.181 -5.181 0.000

MgOH+ 2.401e-007 2.229e-007 -6.620 -6.652 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.380e-008 1.381e-008 -7.860 -7.860 0.000

NaCO3- 3.701e-009 3.436e-009 -8.432 -8.464 -0.032

NaSO4- 3.683e-009 3.419e-009 -8.434 -8.466 -0.032

NaOH 8.647e-012 8.657e-012 -11.063 -11.063 0.000

O(0) 5.264e-004

O2 2.632e-004 2.635e-004 -3.580 -3.579 0.000

S(6) 1.154e-004

SO4-2 9.740e-005 7.271e-005 -4.011 -4.138 -0.127

CaSO4 1.137e-005 1.139e-005 -4.944 -4.944 0.000

MgSO4 6.592e-006 6.599e-006 -5.181 -5.180 0.000

NaSO4- 3.683e-009 3.419e-009 -8.434 -8.466 -0.032

KSO4- 1.751e-009 1.625e-009 -8.757 -8.789 -0.032

HSO4- 5.608e-011 5.207e-011 -10.251 -10.283 -0.032

CaHSO4+ 5.204e-013 4.831e-013 -12.284 -12.316 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.49 -7.85 -8.35 CaCO3

Calcite 0.64 -7.85 -8.49 CaCO3

CO2(g) -2.90 -4.38 -1.49 CO2

Dolomite 1.11 -16.03 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.30 -27.46 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.67 -3.58 -2.91 O2

Initial solution 85. 30/8/2012 08:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.970e-004 4.970e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.150

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 311

Density (g/cm3) = 0.99678

Activity of water = 1.000

Ionic strength = 4.772e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.984e-003

Total CO2 (mol/kg) = 2.984e-003

Temperature (deg C) = 26.800

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551609e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3207 0.7332

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.745e-006 1.618e-006 -5.758 -5.791 -0.033

H+ 7.574e-009 7.079e-009 -8.121 -8.150 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.984e-003

HCO3- 2.847e-003 2.648e-003 -2.546 -2.577 -0.031

CO2 4.122e-005 4.126e-005 -4.385 -4.384 0.000

CaHCO3+ 2.878e-005 2.677e-005 -4.541 -4.572 -0.031

CaCO3 2.443e-005 2.445e-005 -4.612 -4.612 0.000

CO3-2 2.428e-005 1.817e-005 -4.615 -4.741 -0.126

MgHCO3+ 1.244e-005 1.155e-005 -4.905 -4.937 -0.032

MgCO3 6.584e-006 6.591e-006 -5.181 -5.181 0.000

NaHCO3 1.380e-008 1.381e-008 -7.860 -7.860 0.000

NaCO3- 3.701e-009 3.436e-009 -8.432 -8.464 -0.032

Ca 1.096e-003

Ca+2 1.031e-003 7.718e-004 -2.987 -3.113 -0.126

CaHCO3+ 2.878e-005 2.677e-005 -4.541 -4.572 -0.031

CaCO3 2.443e-005 2.445e-005 -4.612 -4.612 0.000

CaSO4 1.137e-005 1.139e-005 -4.944 -4.944 0.000

CaOH+ 1.949e-008 1.809e-008 -7.710 -7.743 -0.032

CaHSO4+ 5.204e-013 4.831e-013 -12.284 -12.316 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 6.963e-028

H2 3.482e-028 3.485e-028 -27.458 -27.458 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.751e-009 1.625e-009 -8.757 -8.789 -0.032

KOH 1.508e-012 1.510e-012 -11.822 -11.821 0.000

Mg 5.184e-004

Mg+2 4.925e-004 3.697e-004 -3.308 -3.432 -0.125

MgHCO3+ 1.244e-005 1.155e-005 -4.905 -4.937 -0.032

MgSO4 6.592e-006 6.599e-006 -5.181 -5.180 0.000

MgCO3 6.584e-006 6.591e-006 -5.181 -5.181 0.000

MgOH+ 2.401e-007 2.229e-007 -6.620 -6.652 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.380e-008 1.381e-008 -7.860 -7.860 0.000

NaCO3- 3.701e-009 3.436e-009 -8.432 -8.464 -0.032

NaSO4- 3.683e-009 3.419e-009 -8.434 -8.466 -0.032

NaOH 8.647e-012 8.657e-012 -11.063 -11.063 0.000

O(0) 4.970e-004

O2 2.485e-004 2.488e-004 -3.605 -3.604 0.000

S(6) 1.154e-004

SO4-2 9.740e-005 7.271e-005 -4.011 -4.138 -0.127

CaSO4 1.137e-005 1.139e-005 -4.944 -4.944 0.000

MgSO4 6.592e-006 6.599e-006 -5.181 -5.180 0.000

NaSO4- 3.683e-009 3.419e-009 -8.434 -8.466 -0.032

KSO4- 1.751e-009 1.625e-009 -8.757 -8.789 -0.032

HSO4- 5.608e-011 5.207e-011 -10.251 -10.283 -0.032

CaHSO4+ 5.204e-013 4.831e-013 -12.284 -12.316 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.49 -7.85 -8.35 CaCO3

Calcite 0.64 -7.85 -8.49 CaCO3

CO2(g) -2.90 -4.38 -1.49 CO2

Dolomite 1.11 -16.03 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.30 -27.46 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.70 -3.60 -2.91 O2

Initial solution 86. 30/8/2012 09:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.283e-004 5.283e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.160

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 312

Density (g/cm3) = 0.99675

Activity of water = 1.000

Ionic strength = 4.770e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.982e-003

Total CO2 (mol/kg) = 2.982e-003

Temperature (deg C) = 26.900

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551611e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3092 0.7328

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.799e-006 1.668e-006 -5.745 -5.778 -0.033

H+ 7.401e-009 6.918e-009 -8.131 -8.160 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.982e-003

HCO3- 2.844e-003 2.645e-003 -2.546 -2.578 -0.031

CO2 4.019e-005 4.024e-005 -4.396 -4.395 0.000

CaHCO3+ 2.877e-005 2.676e-005 -4.541 -4.572 -0.031

CaCO3 2.506e-005 2.509e-005 -4.601 -4.601 0.000

CO3-2 2.486e-005 1.861e-005 -4.604 -4.730 -0.126

MgHCO3+ 1.243e-005 1.154e-005 -4.905 -4.938 -0.032

MgCO3 6.752e-006 6.759e-006 -5.171 -5.170 0.000

NaHCO3 1.378e-008 1.380e-008 -7.861 -7.860 0.000

NaCO3- 3.809e-009 3.536e-009 -8.419 -8.451 -0.032

Ca 1.096e-003

Ca+2 1.031e-003 7.713e-004 -2.987 -3.113 -0.126

CaHCO3+ 2.877e-005 2.676e-005 -4.541 -4.572 -0.031

CaCO3 2.506e-005 2.509e-005 -4.601 -4.601 0.000

CaSO4 1.137e-005 1.139e-005 -4.944 -4.944 0.000

CaOH+ 1.993e-008 1.850e-008 -7.701 -7.733 -0.032

CaHSO4+ 5.093e-013 4.728e-013 -12.293 -12.325 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 6.643e-028

H2 3.322e-028 3.325e-028 -27.479 -27.478 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.753e-009 1.628e-009 -8.756 -8.788 -0.032

KOH 1.543e-012 1.545e-012 -11.812 -11.811 0.000

Mg 5.184e-004

Mg+2 4.924e-004 3.696e-004 -3.308 -3.432 -0.125

MgHCO3+ 1.243e-005 1.154e-005 -4.905 -4.938 -0.032

MgCO3 6.752e-006 6.759e-006 -5.171 -5.170 0.000

MgSO4 6.606e-006 6.613e-006 -5.180 -5.180 0.000

MgOH+ 2.478e-007 2.300e-007 -6.606 -6.638 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.378e-008 1.380e-008 -7.861 -7.860 0.000

NaCO3- 3.809e-009 3.536e-009 -8.419 -8.451 -0.032

NaSO4- 3.685e-009 3.421e-009 -8.434 -8.466 -0.032

NaOH 8.849e-012 8.858e-012 -11.053 -11.053 0.000

O(0) 5.283e-004

O2 2.641e-004 2.644e-004 -3.578 -3.578 0.000

S(6) 1.154e-004

SO4-2 9.738e-005 7.270e-005 -4.012 -4.138 -0.127

CaSO4 1.137e-005 1.139e-005 -4.944 -4.944 0.000

MgSO4 6.606e-006 6.613e-006 -5.180 -5.180 0.000

NaSO4- 3.685e-009 3.421e-009 -8.434 -8.466 -0.032

KSO4- 1.753e-009 1.628e-009 -8.756 -8.788 -0.032

HSO4- 5.492e-011 5.099e-011 -10.260 -10.293 -0.032

CaHSO4+ 5.093e-013 4.728e-013 -12.293 -12.325 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.51 -7.84 -8.35 CaCO3

Calcite 0.65 -7.84 -8.49 CaCO3

CO2(g) -2.91 -4.40 -1.49 CO2

Dolomite 1.13 -16.01 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.32 -27.48 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.67 -3.58 -2.91 O2

Initial solution 87. 30/8/2012 09:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.195e-004 5.195e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.160

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 312

Density (g/cm3) = 0.99675

Activity of water = 1.000

Ionic strength = 4.770e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.982e-003

Total CO2 (mol/kg) = 2.982e-003

Temperature (deg C) = 26.900

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551610e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3074 0.7327

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.799e-006 1.668e-006 -5.745 -5.778 -0.033

H+ 7.401e-009 6.918e-009 -8.131 -8.160 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.982e-003

HCO3- 2.844e-003 2.645e-003 -2.546 -2.578 -0.031

CO2 4.019e-005 4.024e-005 -4.396 -4.395 0.000

CaHCO3+ 2.877e-005 2.676e-005 -4.541 -4.572 -0.031

CaCO3 2.506e-005 2.509e-005 -4.601 -4.601 0.000

CO3-2 2.486e-005 1.861e-005 -4.604 -4.730 -0.126

MgHCO3+ 1.243e-005 1.154e-005 -4.905 -4.938 -0.032

MgCO3 6.752e-006 6.759e-006 -5.171 -5.170 0.000

NaHCO3 1.378e-008 1.380e-008 -7.861 -7.860 0.000

NaCO3- 3.809e-009 3.536e-009 -8.419 -8.451 -0.032

Ca 1.096e-003

Ca+2 1.031e-003 7.713e-004 -2.987 -3.113 -0.126

CaHCO3+ 2.877e-005 2.676e-005 -4.541 -4.572 -0.031

CaCO3 2.506e-005 2.509e-005 -4.601 -4.601 0.000

CaSO4 1.137e-005 1.139e-005 -4.944 -4.944 0.000

CaOH+ 1.993e-008 1.850e-008 -7.701 -7.733 -0.032

CaHSO4+ 5.093e-013 4.728e-013 -12.293 -12.325 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 6.643e-028

H2 3.322e-028 3.325e-028 -27.479 -27.478 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.753e-009 1.628e-009 -8.756 -8.788 -0.032

KOH 1.543e-012 1.545e-012 -11.812 -11.811 0.000

Mg 5.184e-004

Mg+2 4.924e-004 3.696e-004 -3.308 -3.432 -0.125

MgHCO3+ 1.243e-005 1.154e-005 -4.905 -4.938 -0.032

MgCO3 6.752e-006 6.759e-006 -5.171 -5.170 0.000

MgSO4 6.606e-006 6.613e-006 -5.180 -5.180 0.000

MgOH+ 2.478e-007 2.300e-007 -6.606 -6.638 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.378e-008 1.380e-008 -7.861 -7.860 0.000

NaCO3- 3.809e-009 3.536e-009 -8.419 -8.451 -0.032

NaSO4- 3.685e-009 3.421e-009 -8.434 -8.466 -0.032

NaOH 8.849e-012 8.858e-012 -11.053 -11.053 0.000

O(0) 5.195e-004

O2 2.598e-004 2.600e-004 -3.585 -3.585 0.000

S(6) 1.154e-004

SO4-2 9.738e-005 7.270e-005 -4.012 -4.138 -0.127

CaSO4 1.137e-005 1.139e-005 -4.944 -4.944 0.000

MgSO4 6.606e-006 6.613e-006 -5.180 -5.180 0.000

NaSO4- 3.685e-009 3.421e-009 -8.434 -8.466 -0.032

KSO4- 1.753e-009 1.628e-009 -8.756 -8.788 -0.032

HSO4- 5.492e-011 5.099e-011 -10.260 -10.293 -0.032

CaHSO4+ 5.093e-013 4.728e-013 -12.293 -12.325 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.51 -7.84 -8.35 CaCO3

Calcite 0.65 -7.84 -8.49 CaCO3

CO2(g) -2.91 -4.40 -1.49 CO2

Dolomite 1.13 -16.01 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.32 -27.48 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.68 -3.58 -2.91 O2

Initial solution 88. 30/8/2012 09:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.395e-004 4.395e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.180

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 311

Density (g/cm3) = 0.99675

Activity of water = 1.000

Ionic strength = 4.767e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.977e-003

Total CO2 (mol/kg) = 2.977e-003

Temperature (deg C) = 26.900

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551601e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.2692 0.7304

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.883e-006 1.747e-006 -5.725 -5.758 -0.033

H+ 7.068e-009 6.607e-009 -8.151 -8.180 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.977e-003

HCO3- 2.839e-003 2.640e-003 -2.547 -2.578 -0.031

CO2 3.832e-005 3.836e-005 -4.417 -4.416 0.000

CaHCO3+ 2.869e-005 2.669e-005 -4.542 -4.574 -0.031

CaCO3 2.617e-005 2.620e-005 -4.582 -4.582 0.000

CO3-2 2.599e-005 1.946e-005 -4.585 -4.711 -0.126

MgHCO3+ 1.240e-005 1.151e-005 -4.906 -4.939 -0.032

MgCO3 7.054e-006 7.062e-006 -5.152 -5.151 0.000

NaHCO3 1.376e-008 1.377e-008 -7.861 -7.861 0.000

NaCO3- 3.982e-009 3.697e-009 -8.400 -8.432 -0.032

Ca 1.096e-003

Ca+2 1.030e-003 7.706e-004 -2.987 -3.113 -0.126

CaHCO3+ 2.869e-005 2.669e-005 -4.542 -4.574 -0.031

CaCO3 2.617e-005 2.620e-005 -4.582 -4.582 0.000

CaSO4 1.137e-005 1.138e-005 -4.944 -4.944 0.000

CaOH+ 2.085e-008 1.935e-008 -7.681 -7.713 -0.032

CaHSO4+ 4.860e-013 4.512e-013 -12.313 -12.346 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 6.059e-028

H2 3.029e-028 3.033e-028 -27.519 -27.518 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.754e-009 1.628e-009 -8.756 -8.788 -0.032

KOH 1.616e-012 1.618e-012 -11.791 -11.791 0.000

Mg 5.184e-004

Mg+2 4.921e-004 3.694e-004 -3.308 -3.432 -0.125

MgHCO3+ 1.240e-005 1.151e-005 -4.906 -4.939 -0.032

MgCO3 7.054e-006 7.062e-006 -5.152 -5.151 0.000

MgSO4 6.604e-006 6.611e-006 -5.180 -5.180 0.000

MgOH+ 2.593e-007 2.407e-007 -6.586 -6.618 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.376e-008 1.377e-008 -7.861 -7.861 0.000

NaCO3- 3.982e-009 3.697e-009 -8.400 -8.432 -0.032

NaSO4- 3.685e-009 3.421e-009 -8.434 -8.466 -0.032

NaOH 9.266e-012 9.276e-012 -11.033 -11.033 0.000

O(0) 4.395e-004

O2 2.197e-004 2.200e-004 -3.658 -3.658 0.000

S(6) 1.154e-004

SO4-2 9.739e-005 7.271e-005 -4.011 -4.138 -0.127

CaSO4 1.137e-005 1.138e-005 -4.944 -4.944 0.000

MgSO4 6.604e-006 6.611e-006 -5.180 -5.180 0.000

NaSO4- 3.685e-009 3.421e-009 -8.434 -8.466 -0.032

KSO4- 1.754e-009 1.628e-009 -8.756 -8.788 -0.032

HSO4- 5.246e-011 4.870e-011 -10.280 -10.312 -0.032

CaHSO4+ 4.860e-013 4.512e-013 -12.313 -12.346 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.52 -7.82 -8.35 CaCO3

Calcite 0.67 -7.82 -8.49 CaCO3

CO2(g) -2.93 -4.42 -1.49 CO2

Dolomite 1.17 -15.97 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.36 -27.52 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.75 -3.66 -2.91 O2

Initial solution 89. 30/8/2012 09:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.151e-004 5.151e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.170

pe = 4.000

Specific Conductance (uS/cm, 26 oC) = 312

Density (g/cm3) = 0.99675

Activity of water = 1.000

Ionic strength = 4.780e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.990e-003

Total CO2 (mol/kg) = 2.990e-003

Temperature (deg C) = 26.900

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551613e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.2965 0.7320

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.841e-006 1.707e-006 -5.735 -5.768 -0.033

H+ 7.233e-009 6.761e-009 -8.141 -8.170 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.990e-003

HCO3- 2.851e-003 2.652e-003 -2.545 -2.577 -0.031

CO2 3.937e-005 3.942e-005 -4.405 -4.404 0.000

CaHCO3+ 2.892e-005 2.689e-005 -4.539 -4.570 -0.031

CaCO3 2.577e-005 2.580e-005 -4.589 -4.588 0.000

CO3-2 2.551e-005 1.909e-005 -4.593 -4.719 -0.126

MgHCO3+ 1.245e-005 1.156e-005 -4.905 -4.937 -0.032

MgCO3 6.921e-006 6.929e-006 -5.160 -5.159 0.000

NaHCO3 1.382e-008 1.383e-008 -7.860 -7.859 0.000

NaCO3- 3.907e-009 3.627e-009 -8.408 -8.440 -0.032

Ca 1.100e-003

Ca+2 1.034e-003 7.732e-004 -2.986 -3.112 -0.126

CaHCO3+ 2.892e-005 2.689e-005 -4.539 -4.570 -0.031

CaCO3 2.577e-005 2.580e-005 -4.589 -4.588 0.000

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

CaOH+ 2.044e-008 1.898e-008 -7.689 -7.722 -0.032

CaHSO4+ 4.987e-013 4.630e-013 -12.302 -12.334 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 6.344e-028

H2 3.172e-028 3.176e-028 -27.499 -27.498 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.753e-009 1.627e-009 -8.756 -8.789 -0.032

KOH 1.579e-012 1.581e-012 -11.802 -11.801 0.000

Mg 5.184e-004

Mg+2 4.922e-004 3.694e-004 -3.308 -3.433 -0.125

MgHCO3+ 1.245e-005 1.156e-005 -4.905 -4.937 -0.032

MgCO3 6.921e-006 6.929e-006 -5.160 -5.159 0.000

MgSO4 6.598e-006 6.606e-006 -5.181 -5.180 0.000

MgOH+ 2.534e-007 2.352e-007 -6.596 -6.629 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.382e-008 1.383e-008 -7.860 -7.859 0.000

NaCO3- 3.907e-009 3.627e-009 -8.408 -8.440 -0.032

NaSO4- 3.683e-009 3.419e-009 -8.434 -8.466 -0.032

NaOH 9.054e-012 9.064e-012 -11.043 -11.043 0.000

O(0) 5.151e-004

O2 2.576e-004 2.579e-004 -3.589 -3.589 0.000

S(6) 1.154e-004

SO4-2 9.737e-005 7.267e-005 -4.012 -4.139 -0.127

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

MgSO4 6.598e-006 6.606e-006 -5.181 -5.180 0.000

NaSO4- 3.683e-009 3.419e-009 -8.434 -8.466 -0.032

KSO4- 1.753e-009 1.627e-009 -8.756 -8.789 -0.032

HSO4- 5.365e-011 4.980e-011 -10.270 -10.303 -0.032

CaHSO4+ 4.987e-013 4.630e-013 -12.302 -12.334 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.52 -7.83 -8.35 CaCO3

Calcite 0.66 -7.83 -8.49 CaCO3

CO2(g) -2.91 -4.40 -1.49 CO2

Dolomite 1.15 -15.98 -17.13 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.34 -27.50 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.68 -3.59 -2.91 O2

Initial solution 90. 30/8/2012 10:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.011e-003 3.011e-003

Ca 1.100e-003 1.100e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.345e-004 5.345e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.170

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 313

Density (g/cm3) = 0.99673

Activity of water = 1.000

Ionic strength = 4.780e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.989e-003

Total CO2 (mol/kg) = 2.989e-003

Temperature (deg C) = 27.000

Electrical balance (eq) = -4.887e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.78

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551614e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.2923 0.7320

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.854e-006 1.720e-006 -5.732 -5.765 -0.033

H+ 7.233e-009 6.761e-009 -8.141 -8.170 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.989e-003

HCO3- 2.850e-003 2.651e-003 -2.545 -2.577 -0.031

CO2 3.932e-005 3.937e-005 -4.405 -4.405 0.000

CaHCO3+ 2.895e-005 2.692e-005 -4.538 -4.570 -0.031

CaCO3 2.586e-005 2.589e-005 -4.587 -4.587 0.000

CO3-2 2.556e-005 1.913e-005 -4.592 -4.718 -0.126

MgHCO3+ 1.246e-005 1.156e-005 -4.905 -4.937 -0.032

MgCO3 6.943e-006 6.951e-006 -5.158 -5.158 0.000

NaHCO3 1.381e-008 1.383e-008 -7.860 -7.859 0.000

NaCO3- 3.934e-009 3.652e-009 -8.405 -8.438 -0.032

Ca 1.100e-003

Ca+2 1.034e-003 7.731e-004 -2.986 -3.112 -0.126

CaHCO3+ 2.895e-005 2.692e-005 -4.538 -4.570 -0.031

CaCO3 2.586e-005 2.589e-005 -4.587 -4.587 0.000

CaSO4 1.140e-005 1.142e-005 -4.943 -4.942 0.000

CaOH+ 2.044e-008 1.898e-008 -7.689 -7.722 -0.032

CaHSO4+ 4.996e-013 4.638e-013 -12.301 -12.334 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 6.338e-028

H2 3.169e-028 3.173e-028 -27.499 -27.499 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.755e-009 1.629e-009 -8.756 -8.788 -0.032

KOH 1.579e-012 1.581e-012 -11.802 -11.801 0.000

Mg 5.184e-004

Mg+2 4.921e-004 3.693e-004 -3.308 -3.433 -0.125

MgHCO3+ 1.246e-005 1.156e-005 -4.905 -4.937 -0.032

MgCO3 6.943e-006 6.951e-006 -5.158 -5.158 0.000

MgSO4 6.613e-006 6.620e-006 -5.180 -5.179 0.000

MgOH+ 2.556e-007 2.373e-007 -6.592 -6.625 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.381e-008 1.383e-008 -7.860 -7.859 0.000

NaCO3- 3.934e-009 3.652e-009 -8.405 -8.438 -0.032

NaSO4- 3.684e-009 3.420e-009 -8.434 -8.466 -0.032

NaOH 9.054e-012 9.064e-012 -11.043 -11.043 0.000

O(0) 5.345e-004

O2 2.673e-004 2.676e-004 -3.573 -3.573 0.000

S(6) 1.154e-004

SO4-2 9.735e-005 7.265e-005 -4.012 -4.139 -0.127

CaSO4 1.140e-005 1.142e-005 -4.943 -4.942 0.000

MgSO4 6.613e-006 6.620e-006 -5.180 -5.179 0.000

NaSO4- 3.684e-009 3.420e-009 -8.434 -8.466 -0.032

KSO4- 1.755e-009 1.629e-009 -8.756 -8.788 -0.032

HSO4- 5.376e-011 4.990e-011 -10.270 -10.302 -0.032

CaHSO4+ 4.996e-013 4.638e-013 -12.301 -12.334 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.52 -7.83 -8.35 CaCO3

Calcite 0.66 -7.83 -8.49 CaCO3

CO2(g) -2.91 -4.40 -1.49 CO2

Dolomite 1.15 -15.98 -17.14 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.34 -27.50 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.67 -3.57 -2.91 O2

Initial solution 91. 30/8/2012 10:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.021e-003 3.021e-003

Ca 1.104e-003 1.104e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.170e-004 5.170e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.120

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 315

Density (g/cm3) = 0.99670

Activity of water = 1.000

Ionic strength = 4.798e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 3.011e-003

Total CO2 (mol/kg) = 3.011e-003

Temperature (deg C) = 27.100

Electrical balance (eq) = -5.188e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.82

Iterations = 7

Total H = 1.110153e+002

Total O = 5.551619e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.3305 0.7346

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.665e-006 1.544e-006 -5.779 -5.811 -0.033

H+ 8.117e-009 7.586e-009 -8.091 -8.120 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 3.011e-003

HCO3- 2.872e-003 2.671e-003 -2.542 -2.573 -0.032

CO2 4.440e-005 4.445e-005 -4.353 -4.352 0.000

CaHCO3+ 2.935e-005 2.730e-005 -4.532 -4.564 -0.032

CaCO3 2.343e-005 2.346e-005 -4.630 -4.630 0.000

CO3-2 2.300e-005 1.721e-005 -4.638 -4.764 -0.126

MgHCO3+ 1.257e-005 1.166e-005 -4.901 -4.933 -0.032

MgCO3 6.260e-006 6.267e-006 -5.203 -5.203 0.000

NaHCO3 1.391e-008 1.393e-008 -7.857 -7.856 0.000

NaCO3- 3.557e-009 3.301e-009 -8.449 -8.481 -0.032

Ca 1.104e-003

Ca+2 1.039e-003 7.769e-004 -2.983 -3.110 -0.126

CaHCO3+ 2.935e-005 2.730e-005 -4.532 -4.564 -0.032

CaCO3 2.343e-005 2.346e-005 -4.630 -4.630 0.000

CaSO4 1.146e-005 1.147e-005 -4.941 -4.940 0.000

CaOH+ 1.831e-008 1.700e-008 -7.737 -7.770 -0.032

CaHSO4+ 5.640e-013 5.235e-013 -12.249 -12.281 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.312e-005 -4.242 -4.275 -0.033

H(0) 7.971e-028

H2 3.986e-028 3.990e-028 -27.399 -27.399 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.756e-009 1.630e-009 -8.755 -8.788 -0.032

KOH 1.407e-012 1.409e-012 -11.852 -11.851 0.000

Mg 5.184e-004

Mg+2 4.927e-004 3.696e-004 -3.307 -3.432 -0.125

MgHCO3+ 1.257e-005 1.166e-005 -4.901 -4.933 -0.032

MgSO4 6.626e-006 6.633e-006 -5.179 -5.178 0.000

MgCO3 6.260e-006 6.267e-006 -5.203 -5.203 0.000

MgOH+ 2.300e-007 2.135e-007 -6.638 -6.671 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.391e-008 1.393e-008 -7.857 -7.856 0.000

NaSO4- 3.682e-009 3.418e-009 -8.434 -8.466 -0.032

NaCO3- 3.557e-009 3.301e-009 -8.449 -8.481 -0.032

NaOH 8.068e-012 8.077e-012 -11.093 -11.093 0.000

O(0) 5.170e-004

O2 2.585e-004 2.588e-004 -3.588 -3.587 0.000

S(6) 1.154e-004

SO4-2 9.728e-005 7.256e-005 -4.012 -4.139 -0.127

CaSO4 1.146e-005 1.147e-005 -4.941 -4.940 0.000

MgSO4 6.626e-006 6.633e-006 -5.179 -5.178 0.000

NaSO4- 3.682e-009 3.418e-009 -8.434 -8.466 -0.032

KSO4- 1.756e-009 1.630e-009 -8.755 -8.788 -0.032

HSO4- 6.038e-011 5.604e-011 -10.219 -10.251 -0.032

CaHSO4+ 5.640e-013 5.235e-013 -12.249 -12.281 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.48 -7.87 -8.35 CaCO3

Calcite 0.62 -7.87 -8.49 CaCO3

CO2(g) -2.86 -4.35 -1.49 CO2

Dolomite 1.07 -16.07 -17.14 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.24 -27.40 -3.16 H2

H2O(g) -1.46 -0.00 1.46 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.68 -3.59 -2.91 O2

Initial solution 92. 30/8/2012 10:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.358e-004 5.358e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.180

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 313

Density (g/cm3) = 0.99667

Activity of water = 1.000

Ionic strength = 4.765e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.977e-003

Total CO2 (mol/kg) = 2.977e-003

Temperature (deg C) = 27.200

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551611e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.2662 0.7310

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.926e-006 1.786e-006 -5.715 -5.748 -0.033

H+ 7.068e-009 6.607e-009 -8.151 -8.180 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.977e-003

HCO3- 2.837e-003 2.639e-003 -2.547 -2.579 -0.031

CO2 3.817e-005 3.821e-005 -4.418 -4.418 0.000

CaHCO3+ 2.879e-005 2.678e-005 -4.541 -4.572 -0.031

CaCO3 2.646e-005 2.649e-005 -4.577 -4.577 0.000

CO3-2 2.613e-005 1.956e-005 -4.583 -4.709 -0.126

MgHCO3+ 1.241e-005 1.152e-005 -4.906 -4.938 -0.032

MgCO3 7.122e-006 7.129e-006 -5.147 -5.147 0.000

NaHCO3 1.375e-008 1.377e-008 -7.862 -7.861 0.000

NaCO3- 4.063e-009 3.772e-009 -8.391 -8.423 -0.032

Ca 1.096e-003

Ca+2 1.029e-003 7.702e-004 -2.987 -3.113 -0.126

CaHCO3+ 2.879e-005 2.678e-005 -4.541 -4.572 -0.031

CaCO3 2.646e-005 2.649e-005 -4.577 -4.577 0.000

CaSO4 1.138e-005 1.140e-005 -4.944 -4.943 0.000

CaOH+ 2.084e-008 1.934e-008 -7.681 -7.713 -0.032

CaHSO4+ 4.886e-013 4.536e-013 -12.311 -12.343 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 6.041e-028

H2 3.021e-028 3.024e-028 -27.520 -27.519 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.761e-009 1.635e-009 -8.754 -8.786 -0.032

KOH 1.616e-012 1.618e-012 -11.792 -11.791 0.000

Mg 5.184e-004

Mg+2 4.920e-004 3.693e-004 -3.308 -3.433 -0.125

MgHCO3+ 1.241e-005 1.152e-005 -4.906 -4.938 -0.032

MgCO3 7.122e-006 7.129e-006 -5.147 -5.147 0.000

MgSO4 6.647e-006 6.654e-006 -5.177 -5.177 0.000

MgOH+ 2.662e-007 2.472e-007 -6.575 -6.607 -0.032

Na 1.001e-005

Na+ 9.986e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.375e-008 1.377e-008 -7.862 -7.861 0.000

NaCO3- 4.063e-009 3.772e-009 -8.391 -8.423 -0.032

NaSO4- 3.689e-009 3.425e-009 -8.433 -8.465 -0.032

NaOH 9.265e-012 9.275e-012 -11.033 -11.033 0.000

O(0) 5.358e-004

O2 2.679e-004 2.682e-004 -3.572 -3.572 0.000

S(6) 1.154e-004

SO4-2 9.733e-005 7.266e-005 -4.012 -4.139 -0.127

CaSO4 1.138e-005 1.140e-005 -4.944 -4.943 0.000

MgSO4 6.647e-006 6.654e-006 -5.177 -5.177 0.000

NaSO4- 3.689e-009 3.425e-009 -8.433 -8.465 -0.032

KSO4- 1.761e-009 1.635e-009 -8.754 -8.786 -0.032

HSO4- 5.277e-011 4.899e-011 -10.278 -10.310 -0.032

CaHSO4+ 4.886e-013 4.536e-013 -12.311 -12.343 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.53 -7.82 -8.35 CaCO3

Calcite 0.67 -7.82 -8.49 CaCO3

CO2(g) -2.92 -4.42 -1.49 CO2

Dolomite 1.18 -15.96 -17.14 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.36 -27.52 -3.16 H2

H2O(g) -1.45 -0.00 1.45 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.66 -3.57 -2.91 O2

Initial solution 93. 30/8/2012 10:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 3.000e-003 3.000e-003

Ca 1.096e-003 1.096e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.289e-004 5.289e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.220

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 315

Density (g/cm3) = 0.99659

Activity of water = 1.000

Ionic strength = 4.758e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.967e-003

Total CO2 (mol/kg) = 2.967e-003

Temperature (deg C) = 27.500

Electrical balance (eq) = -4.603e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551608e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.2003 0.7278

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.159e-006 2.002e-006 -5.666 -5.699 -0.033

H+ 6.446e-009 6.026e-009 -8.191 -8.220 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.967e-003

HCO3- 2.825e-003 2.628e-003 -2.549 -2.580 -0.031

CO2 3.455e-005 3.459e-005 -4.462 -4.461 0.000

CaCO3 2.918e-005 2.921e-005 -4.535 -4.535 0.000

CaHCO3+ 2.871e-005 2.671e-005 -4.542 -4.573 -0.031

CO3-2 2.869e-005 2.148e-005 -4.542 -4.668 -0.126

MgHCO3+ 1.236e-005 1.147e-005 -4.908 -4.940 -0.032

MgCO3 7.844e-006 7.853e-006 -5.105 -5.105 0.000

NaHCO3 1.369e-008 1.371e-008 -7.863 -7.863 0.000

NaCO3- 4.528e-009 4.204e-009 -8.344 -8.376 -0.032

Ca 1.096e-003

Ca+2 1.027e-003 7.683e-004 -2.989 -3.114 -0.126

CaCO3 2.918e-005 2.921e-005 -4.535 -4.535 0.000

CaHCO3+ 2.871e-005 2.671e-005 -4.542 -4.573 -0.031

CaSO4 1.138e-005 1.140e-005 -4.944 -4.943 0.000

CaOH+ 2.279e-008 2.116e-008 -7.642 -7.675 -0.032

CaHSO4+ 4.473e-013 4.153e-013 -12.349 -12.382 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 5.010e-028

H2 2.505e-028 2.508e-028 -27.601 -27.601 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.770e-009 1.643e-009 -8.752 -8.784 -0.032

KOH 1.772e-012 1.774e-012 -11.752 -11.751 0.000

Mg 5.184e-004

Mg+2 4.912e-004 3.688e-004 -3.309 -3.433 -0.125

MgHCO3+ 1.236e-005 1.147e-005 -4.908 -4.940 -0.032

MgCO3 7.844e-006 7.853e-006 -5.105 -5.105 0.000

MgSO4 6.686e-006 6.693e-006 -5.175 -5.174 0.000

MgOH+ 2.994e-007 2.779e-007 -6.524 -6.556 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.369e-008 1.371e-008 -7.863 -7.863 0.000

NaCO3- 4.528e-009 4.204e-009 -8.344 -8.376 -0.032

NaSO4- 3.695e-009 3.430e-009 -8.432 -8.465 -0.032

NaOH 1.016e-011 1.017e-011 -10.993 -10.993 0.000

O(0) 5.289e-004

O2 2.644e-004 2.647e-004 -3.578 -3.577 0.000

S(6) 1.154e-004

SO4-2 9.730e-005 7.264e-005 -4.012 -4.139 -0.127

CaSO4 1.138e-005 1.140e-005 -4.944 -4.943 0.000

MgSO4 6.686e-006 6.693e-006 -5.175 -5.174 0.000

NaSO4- 3.695e-009 3.430e-009 -8.432 -8.465 -0.032

KSO4- 1.770e-009 1.643e-009 -8.752 -8.784 -0.032

HSO4- 4.843e-011 4.496e-011 -10.315 -10.347 -0.032

CaHSO4+ 4.473e-013 4.153e-013 -12.349 -12.382 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.57 -7.78 -8.35 CaCO3

Calcite 0.71 -7.78 -8.49 CaCO3

CO2(g) -2.96 -4.46 -1.50 CO2

Dolomite 1.26 -15.88 -17.15 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.44 -27.60 -3.16 H2

H2O(g) -1.45 -0.00 1.45 H2O

Halite -10.89 -9.31 1.59 NaCl

O2(g) -0.67 -3.58 -2.91 O2

Initial solution 94. 30/8/2012 11:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.980e-003 2.980e-003

Ca 1.089e-003 1.089e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.508e-004 5.508e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.220

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 315

Density (g/cm3) = 0.99653

Activity of water = 1.000

Ionic strength = 4.733e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.946e-003

Total CO2 (mol/kg) = 2.946e-003

Temperature (deg C) = 27.700

Electrical balance (eq) = -4.035e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.65

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551604e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1885 0.7275

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.190e-006 2.032e-006 -5.659 -5.692 -0.033

H+ 6.445e-009 6.026e-009 -8.191 -8.220 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.946e-003

HCO3- 2.806e-003 2.610e-003 -2.552 -2.583 -0.031

CO2 3.424e-005 3.428e-005 -4.465 -4.465 0.000

CaCO3 2.903e-005 2.906e-005 -4.537 -4.537 0.000

CO3-2 2.858e-005 2.141e-005 -4.544 -4.669 -0.125

CaHCO3+ 2.841e-005 2.643e-005 -4.547 -4.578 -0.031

MgHCO3+ 1.229e-005 1.141e-005 -4.910 -4.943 -0.032

MgCO3 7.849e-006 7.857e-006 -5.105 -5.105 0.000

NaHCO3 1.360e-008 1.362e-008 -7.866 -7.866 0.000

NaCO3- 4.559e-009 4.233e-009 -8.341 -8.373 -0.032

Ca 1.089e-003

Ca+2 1.020e-003 7.635e-004 -2.991 -3.117 -0.126

CaCO3 2.903e-005 2.906e-005 -4.537 -4.537 0.000

CaHCO3+ 2.841e-005 2.643e-005 -4.547 -4.578 -0.031

CaSO4 1.134e-005 1.135e-005 -4.945 -4.945 0.000

CaOH+ 2.264e-008 2.103e-008 -7.645 -7.677 -0.032

CaHSO4+ 4.467e-013 4.148e-013 -12.350 -12.382 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 5.000e-028

H2 2.500e-028 2.503e-028 -27.602 -27.602 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.777e-009 1.650e-009 -8.750 -8.783 -0.032

KOH 1.772e-012 1.774e-012 -11.751 -11.751 0.000

Mg 5.184e-004

Mg+2 4.912e-004 3.690e-004 -3.309 -3.433 -0.124

MgHCO3+ 1.229e-005 1.141e-005 -4.910 -4.943 -0.032

MgCO3 7.849e-006 7.857e-006 -5.105 -5.105 0.000

MgSO4 6.727e-006 6.735e-006 -5.172 -5.172 0.000

MgOH+ 3.049e-007 2.831e-007 -6.516 -6.548 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.360e-008 1.362e-008 -7.866 -7.866 0.000

NaCO3- 4.559e-009 4.233e-009 -8.341 -8.373 -0.032

NaSO4- 3.702e-009 3.437e-009 -8.432 -8.464 -0.032

NaOH 1.016e-011 1.017e-011 -10.993 -10.993 0.000

O(0) 5.508e-004

O2 2.754e-004 2.757e-004 -3.560 -3.560 0.000

S(6) 1.154e-004

SO4-2 9.730e-005 7.268e-005 -4.012 -4.139 -0.127

CaSO4 1.134e-005 1.135e-005 -4.945 -4.945 0.000

MgSO4 6.727e-006 6.735e-006 -5.172 -5.172 0.000

NaSO4- 3.702e-009 3.437e-009 -8.432 -8.464 -0.032

KSO4- 1.777e-009 1.650e-009 -8.750 -8.783 -0.032

HSO4- 4.867e-011 4.519e-011 -10.313 -10.345 -0.032

CaHSO4+ 4.467e-013 4.148e-013 -12.350 -12.382 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.37 CaSO4

Aragonite 0.57 -7.79 -8.35 CaCO3

Calcite 0.71 -7.79 -8.50 CaCO3

CO2(g) -2.97 -4.47 -1.50 CO2

Dolomite 1.26 -15.89 -17.15 CaMg(CO3)2

Gypsum -2.67 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.44 -27.60 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.65 -3.56 -2.91 O2

Initial solution 95. 30/8/2012 11:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.980e-003 2.980e-003

Ca 1.089e-003 1.089e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.589e-004 5.589e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.220

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 315

Density (g/cm3) = 0.99650

Activity of water = 1.000

Ionic strength = 4.733e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.946e-003

Total CO2 (mol/kg) = 2.946e-003

Temperature (deg C) = 27.800

Electrical balance (eq) = -4.035e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.65

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551604e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1819 0.7274

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.207e-006 2.047e-006 -5.656 -5.689 -0.033

H+ 6.445e-009 6.026e-009 -8.191 -8.220 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.946e-003

HCO3- 2.805e-003 2.610e-003 -2.552 -2.583 -0.031

CO2 3.420e-005 3.423e-005 -4.466 -4.466 0.000

CaCO3 2.914e-005 2.917e-005 -4.536 -4.535 0.000

CO3-2 2.863e-005 2.145e-005 -4.543 -4.669 -0.126

CaHCO3+ 2.844e-005 2.646e-005 -4.546 -4.577 -0.031

MgHCO3+ 1.229e-005 1.142e-005 -4.910 -4.943 -0.032

MgCO3 7.873e-006 7.882e-006 -5.104 -5.103 0.000

NaHCO3 1.360e-008 1.361e-008 -7.866 -7.866 0.000

NaCO3- 4.589e-009 4.261e-009 -8.338 -8.370 -0.032

Ca 1.089e-003

Ca+2 1.020e-003 7.633e-004 -2.992 -3.117 -0.126

CaCO3 2.914e-005 2.917e-005 -4.536 -4.535 0.000

CaHCO3+ 2.844e-005 2.646e-005 -4.546 -4.577 -0.031

CaSO4 1.134e-005 1.136e-005 -4.945 -4.945 0.000

CaOH+ 2.264e-008 2.102e-008 -7.645 -7.677 -0.032

CaHSO4+ 4.475e-013 4.155e-013 -12.349 -12.381 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 4.995e-028

H2 2.498e-028 2.500e-028 -27.602 -27.602 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.780e-009 1.652e-009 -8.750 -8.782 -0.032

KOH 1.772e-012 1.774e-012 -11.751 -11.751 0.000

Mg 5.184e-004

Mg+2 4.912e-004 3.689e-004 -3.309 -3.433 -0.124

MgHCO3+ 1.229e-005 1.142e-005 -4.910 -4.943 -0.032

MgCO3 7.873e-006 7.882e-006 -5.104 -5.103 0.000

MgSO4 6.742e-006 6.749e-006 -5.171 -5.171 0.000

MgOH+ 3.075e-007 2.856e-007 -6.512 -6.544 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.360e-008 1.361e-008 -7.866 -7.866 0.000

NaCO3- 4.589e-009 4.261e-009 -8.338 -8.370 -0.032

NaSO4- 3.703e-009 3.438e-009 -8.431 -8.464 -0.032

NaOH 1.016e-011 1.017e-011 -10.993 -10.993 0.000

O(0) 5.589e-004

O2 2.794e-004 2.798e-004 -3.554 -3.553 0.000

S(6) 1.154e-004

SO4-2 9.728e-005 7.266e-005 -4.012 -4.139 -0.127

CaSO4 1.134e-005 1.136e-005 -4.945 -4.945 0.000

MgSO4 6.742e-006 6.749e-006 -5.171 -5.171 0.000

NaSO4- 3.703e-009 3.438e-009 -8.431 -8.464 -0.032

KSO4- 1.780e-009 1.652e-009 -8.750 -8.782 -0.032

HSO4- 4.877e-011 4.528e-011 -10.312 -10.344 -0.032

CaHSO4+ 4.475e-013 4.155e-013 -12.349 -12.381 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.37 CaSO4

Aragonite 0.57 -7.79 -8.35 CaCO3

Calcite 0.71 -7.79 -8.50 CaCO3

CO2(g) -2.97 -4.47 -1.50 CO2

Dolomite 1.27 -15.89 -17.15 CaMg(CO3)2

Gypsum -2.67 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.44 -27.60 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.64 -3.55 -2.91 O2

Initial solution 96. 30/8/2012 11:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.980e-003 2.980e-003

Ca 1.089e-003 1.089e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.676e-004 5.676e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.200

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 315

Density (g/cm3) = 0.99653

Activity of water = 1.000

Ionic strength = 4.737e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.951e-003

Total CO2 (mol/kg) = 2.951e-003

Temperature (deg C) = 27.700

Electrical balance (eq) = -4.035e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.65

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551606e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.2117 0.7289

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.092e-006 1.940e-006 -5.679 -5.712 -0.033

H+ 6.749e-009 6.310e-009 -8.171 -8.200 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.951e-003

HCO3- 2.811e-003 2.615e-003 -2.551 -2.583 -0.031

CO2 3.592e-005 3.596e-005 -4.445 -4.444 0.000

CaHCO3+ 2.850e-005 2.651e-005 -4.545 -4.577 -0.031

CaCO3 2.780e-005 2.784e-005 -4.556 -4.555 0.000

CO3-2 2.735e-005 2.049e-005 -4.563 -4.689 -0.126

MgHCO3+ 1.232e-005 1.144e-005 -4.909 -4.942 -0.032

MgCO3 7.514e-006 7.522e-006 -5.124 -5.124 0.000

NaHCO3 1.363e-008 1.364e-008 -7.866 -7.865 0.000

NaCO3- 4.362e-009 4.050e-009 -8.360 -8.393 -0.032

Ca 1.089e-003

Ca+2 1.021e-003 7.642e-004 -2.991 -3.117 -0.126

CaHCO3+ 2.850e-005 2.651e-005 -4.545 -4.577 -0.031

CaCO3 2.780e-005 2.784e-005 -4.556 -4.555 0.000

CaSO4 1.135e-005 1.136e-005 -4.945 -4.945 0.000

CaOH+ 2.165e-008 2.010e-008 -7.665 -7.697 -0.032

CaHSO4+ 4.682e-013 4.347e-013 -12.330 -12.362 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 5.483e-028

H2 2.741e-028 2.744e-028 -27.562 -27.562 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.777e-009 1.650e-009 -8.750 -8.783 -0.032

KOH 1.693e-012 1.694e-012 -11.771 -11.771 0.000

Mg 5.184e-004

Mg+2 4.915e-004 3.692e-004 -3.308 -3.433 -0.124

MgHCO3+ 1.232e-005 1.144e-005 -4.909 -4.942 -0.032

MgCO3 7.514e-006 7.522e-006 -5.124 -5.124 0.000

MgSO4 6.730e-006 6.737e-006 -5.172 -5.172 0.000

MgOH+ 2.913e-007 2.705e-007 -6.536 -6.568 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.363e-008 1.364e-008 -7.866 -7.865 0.000

NaCO3- 4.362e-009 4.050e-009 -8.360 -8.393 -0.032

NaSO4- 3.701e-009 3.436e-009 -8.432 -8.464 -0.032

NaOH 9.703e-012 9.714e-012 -11.013 -11.013 0.000

O(0) 5.676e-004

O2 2.838e-004 2.841e-004 -3.547 -3.546 0.000

S(6) 1.154e-004

SO4-2 9.729e-005 7.266e-005 -4.012 -4.139 -0.127

CaSO4 1.135e-005 1.136e-005 -4.945 -4.945 0.000

MgSO4 6.730e-006 6.737e-006 -5.172 -5.172 0.000

NaSO4- 3.701e-009 3.436e-009 -8.432 -8.464 -0.032

KSO4- 1.777e-009 1.650e-009 -8.750 -8.783 -0.032

HSO4- 5.095e-011 4.731e-011 -10.293 -10.325 -0.032

CaHSO4+ 4.682e-013 4.347e-013 -12.330 -12.362 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.37 CaSO4

Aragonite 0.55 -7.81 -8.35 CaCO3

Calcite 0.69 -7.81 -8.50 CaCO3

CO2(g) -2.95 -4.44 -1.50 CO2

Dolomite 1.23 -15.93 -17.15 CaMg(CO3)2

Gypsum -2.67 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.40 -27.56 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.64 -3.55 -2.91 O2

Initial solution 97. 30/8/2012 11:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.990e-003 2.990e-003

Ca 1.092e-003 1.092e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.651e-004 5.651e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.200

pe = 4.000

Specific Conductance (uS/cm, 27 oC) = 317

Density (g/cm3) = 0.99647

Activity of water = 1.000

Ionic strength = 4.747e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.960e-003

Total CO2 (mol/kg) = 2.960e-003

Temperature (deg C) = 27.900

Electrical balance (eq) = -4.336e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.70

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551609e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1950 0.7284

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.123e-006 1.969e-006 -5.673 -5.706 -0.033

H+ 6.750e-009 6.310e-009 -8.171 -8.200 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.960e-003

HCO3- 2.820e-003 2.623e-003 -2.550 -2.581 -0.031

CO2 3.596e-005 3.599e-005 -4.444 -4.444 0.000

CaHCO3+ 2.874e-005 2.673e-005 -4.542 -4.573 -0.031

CaCO3 2.819e-005 2.822e-005 -4.550 -4.549 0.000

CO3-2 2.755e-005 2.063e-005 -4.560 -4.686 -0.126

MgHCO3+ 1.237e-005 1.148e-005 -4.908 -4.940 -0.032

MgCO3 7.584e-006 7.592e-006 -5.120 -5.120 0.000

NaHCO3 1.367e-008 1.368e-008 -7.864 -7.864 0.000

NaCO3- 4.436e-009 4.118e-009 -8.353 -8.385 -0.032

Ca 1.092e-003

Ca+2 1.024e-003 7.662e-004 -2.990 -3.116 -0.126

CaHCO3+ 2.874e-005 2.673e-005 -4.542 -4.573 -0.031

CaCO3 2.819e-005 2.822e-005 -4.550 -4.549 0.000

CaSO4 1.139e-005 1.140e-005 -4.944 -4.943 0.000

CaOH+ 2.171e-008 2.015e-008 -7.663 -7.696 -0.032

CaHSO4+ 4.711e-013 4.373e-013 -12.327 -12.359 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 5.472e-028

H2 2.736e-028 2.739e-028 -27.563 -27.562 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.781e-009 1.653e-009 -8.749 -8.782 -0.032

KOH 1.692e-012 1.694e-012 -11.771 -11.771 0.000

Mg 5.184e-004

Mg+2 4.914e-004 3.689e-004 -3.309 -3.433 -0.124

MgHCO3+ 1.237e-005 1.148e-005 -4.908 -4.940 -0.032

MgCO3 7.584e-006 7.592e-006 -5.120 -5.120 0.000

MgSO4 6.752e-006 6.760e-006 -5.171 -5.170 0.000

MgOH+ 2.963e-007 2.751e-007 -6.528 -6.560 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.367e-008 1.368e-008 -7.864 -7.864 0.000

NaCO3- 4.436e-009 4.118e-009 -8.353 -8.385 -0.032

NaSO4- 3.702e-009 3.437e-009 -8.432 -8.464 -0.032

NaOH 9.702e-012 9.713e-012 -11.013 -11.013 0.000

O(0) 5.651e-004

O2 2.826e-004 2.829e-004 -3.549 -3.548 0.000

S(6) 1.154e-004

SO4-2 9.722e-005 7.259e-005 -4.012 -4.139 -0.127

CaSO4 1.139e-005 1.140e-005 -4.944 -4.943 0.000

MgSO4 6.752e-006 6.760e-006 -5.171 -5.170 0.000

NaSO4- 3.702e-009 3.437e-009 -8.432 -8.464 -0.032

KSO4- 1.781e-009 1.653e-009 -8.749 -8.782 -0.032

HSO4- 5.113e-011 4.747e-011 -10.291 -10.324 -0.032

CaHSO4+ 4.711e-013 4.373e-013 -12.327 -12.359 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.25 -4.37 CaSO4

Aragonite 0.55 -7.80 -8.36 CaCO3

Calcite 0.70 -7.80 -8.50 CaCO3

CO2(g) -2.94 -4.44 -1.50 CO2

Dolomite 1.24 -15.92 -17.16 CaMg(CO3)2

Gypsum -2.67 -7.25 -4.58 CaSO4:2H2O

H2(g) -24.40 -27.56 -3.16 H2

H2O(g) -1.44 -0.00 1.44 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.64 -3.55 -2.91 O2

Initial solution 98. 30/8/2012 12:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.990e-003 2.990e-003

Ca 1.092e-003 1.092e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.820e-004 5.820e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.240

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 319

Density (g/cm3) = 0.99639

Activity of water = 1.000

Ionic strength = 4.739e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.950e-003

Total CO2 (mol/kg) = 2.950e-003

Temperature (deg C) = 28.200

Electrical balance (eq) = -4.336e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.70

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551608e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.1338 0.7255

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.379e-006 2.207e-006 -5.624 -5.656 -0.033

H+ 6.156e-009 5.754e-009 -8.211 -8.240 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.950e-003

HCO3- 2.807e-003 2.611e-003 -2.552 -2.583 -0.031

CO2 3.254e-005 3.258e-005 -4.488 -4.487 0.000

CaCO3 3.107e-005 3.110e-005 -4.508 -4.507 0.000

CO3-2 3.024e-005 2.264e-005 -4.519 -4.645 -0.126

CaHCO3+ 2.865e-005 2.665e-005 -4.543 -4.574 -0.031

MgHCO3+ 1.231e-005 1.143e-005 -4.910 -4.942 -0.032

MgCO3 8.350e-006 8.359e-006 -5.078 -5.078 0.000

NaHCO3 1.361e-008 1.362e-008 -7.866 -7.866 0.000

NaCO3- 4.941e-009 4.587e-009 -8.306 -8.338 -0.032

Ca 1.092e-003

Ca+2 1.021e-003 7.642e-004 -2.991 -3.117 -0.126

CaCO3 3.107e-005 3.110e-005 -4.508 -4.507 0.000

CaHCO3+ 2.865e-005 2.665e-005 -4.543 -4.574 -0.031

CaSO4 1.138e-005 1.140e-005 -4.944 -4.943 0.000

CaOH+ 2.374e-008 2.204e-008 -7.625 -7.657 -0.032

CaHSO4+ 4.312e-013 4.004e-013 -12.365 -12.398 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.313e-005 -4.242 -4.275 -0.033

H(0) 4.538e-028

H2 2.269e-028 2.271e-028 -27.644 -27.644 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.790e-009 1.661e-009 -8.747 -8.780 -0.032

KOH 1.856e-012 1.858e-012 -11.731 -11.731 0.000

Mg 5.184e-004

Mg+2 4.906e-004 3.684e-004 -3.309 -3.434 -0.124

MgHCO3+ 1.231e-005 1.143e-005 -4.910 -4.942 -0.032

MgCO3 8.350e-006 8.359e-006 -5.078 -5.078 0.000

MgSO4 6.791e-006 6.799e-006 -5.168 -5.168 0.000

MgOH+ 3.332e-007 3.093e-007 -6.477 -6.510 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.361e-008 1.362e-008 -7.866 -7.866 0.000

NaCO3- 4.941e-009 4.587e-009 -8.306 -8.338 -0.032

NaSO4- 3.707e-009 3.442e-009 -8.431 -8.463 -0.032

NaOH 1.064e-011 1.065e-011 -10.973 -10.973 0.000

O(0) 5.820e-004

O2 2.910e-004 2.913e-004 -3.536 -3.536 0.000

S(6) 1.154e-004

SO4-2 9.719e-005 7.257e-005 -4.012 -4.139 -0.127

CaSO4 1.138e-005 1.140e-005 -4.944 -4.943 0.000

MgSO4 6.791e-006 6.799e-006 -5.168 -5.168 0.000

NaSO4- 3.707e-009 3.442e-009 -8.431 -8.463 -0.032

KSO4- 1.790e-009 1.661e-009 -8.747 -8.780 -0.032

HSO4- 4.693e-011 4.357e-011 -10.329 -10.361 -0.032

CaHSO4+ 4.312e-013 4.004e-013 -12.365 -12.398 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.60 -7.76 -8.36 CaCO3

Calcite 0.74 -7.76 -8.50 CaCO3

CO2(g) -2.98 -4.49 -1.50 CO2

Dolomite 1.32 -15.84 -17.16 CaMg(CO3)2

Gypsum -2.67 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.48 -27.64 -3.16 H2

H2O(g) -1.43 -0.00 1.43 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.62 -3.54 -2.91 O2

Initial solution 99. 30/8/2012 12:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.139e-004 6.139e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.270

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 317

Density (g/cm3) = 0.99633

Activity of water = 1.000

Ionic strength = 4.698e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.912e-003

Total CO2 (mol/kg) = 2.912e-003

Temperature (deg C) = 28.400

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551600e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.0934 0.7236

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.586e-006 2.400e-006 -5.587 -5.620 -0.033

H+ 5.744e-009 5.370e-009 -8.241 -8.270 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.912e-003

HCO3- 2.769e-003 2.576e-003 -2.558 -2.589 -0.031

CaCO3 3.275e-005 3.278e-005 -4.485 -4.484 0.000

CO3-2 3.205e-005 2.402e-005 -4.494 -4.619 -0.125

CO2 2.990e-005 2.993e-005 -4.524 -4.524 0.000

CaHCO3+ 2.802e-005 2.607e-005 -4.553 -4.584 -0.031

MgHCO3+ 1.215e-005 1.129e-005 -4.915 -4.947 -0.032

MgCO3 8.887e-006 8.896e-006 -5.051 -5.051 0.000

NaHCO3 1.343e-008 1.344e-008 -7.872 -7.872 0.000

NaCO3- 5.294e-009 4.917e-009 -8.276 -8.308 -0.032

Ca 1.081e-003

Ca+2 1.009e-003 7.559e-004 -2.996 -3.122 -0.125

CaCO3 3.275e-005 3.278e-005 -4.485 -4.484 0.000

CaHCO3+ 2.802e-005 2.607e-005 -4.553 -4.584 -0.031

CaSO4 1.130e-005 1.131e-005 -4.947 -4.947 0.000

CaOH+ 2.515e-008 2.336e-008 -7.599 -7.632 -0.032

CaHSO4+ 4.003e-013 3.718e-013 -12.398 -12.430 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.275 -0.032

H(0) 3.945e-028

H2 1.972e-028 1.975e-028 -27.705 -27.705 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.798e-009 1.670e-009 -8.745 -8.777 -0.032

KOH 1.989e-012 1.991e-012 -11.701 -11.701 0.000

Mg 5.184e-004

Mg+2 4.902e-004 3.684e-004 -3.310 -3.434 -0.124

MgHCO3+ 1.215e-005 1.129e-005 -4.915 -4.947 -0.032

MgCO3 8.887e-006 8.896e-006 -5.051 -5.051 0.000

MgSO4 6.836e-006 6.844e-006 -5.165 -5.165 0.000

MgOH+ 3.633e-007 3.374e-007 -6.440 -6.472 -0.032

Na 1.001e-005

Na+ 9.985e-006 9.278e-006 -5.001 -5.033 -0.032

NaHCO3 1.343e-008 1.344e-008 -7.872 -7.872 0.000

NaCO3- 5.294e-009 4.917e-009 -8.276 -8.308 -0.032

NaSO4- 3.717e-009 3.452e-009 -8.430 -8.462 -0.032

NaOH 1.140e-011 1.141e-011 -10.943 -10.943 0.000

O(0) 6.139e-004

O2 3.070e-004 3.073e-004 -3.513 -3.512 0.000

S(6) 1.154e-004

SO4-2 9.723e-005 7.267e-005 -4.012 -4.139 -0.126

CaSO4 1.130e-005 1.131e-005 -4.947 -4.947 0.000

MgSO4 6.836e-006 6.844e-006 -5.165 -5.165 0.000

NaSO4- 3.717e-009 3.452e-009 -8.430 -8.462 -0.032

KSO4- 1.798e-009 1.670e-009 -8.745 -8.777 -0.032

HSO4- 4.405e-011 4.091e-011 -10.356 -10.388 -0.032

CaHSO4+ 4.003e-013 3.718e-013 -12.398 -12.430 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.62 -7.74 -8.36 CaCO3

Calcite 0.76 -7.74 -8.50 CaCO3

CO2(g) -3.02 -4.52 -1.51 CO2

Dolomite 1.37 -15.79 -17.17 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.54 -27.70 -3.16 H2

H2O(g) -1.42 -0.00 1.42 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.60 -3.51 -2.92 O2

Initial solution 100. 30/8/2012 12:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.980e-003 2.980e-003

Ca 1.089e-003 1.089e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.839e-004 5.839e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.300

pe = 4.000

Specific Conductance (uS/cm, 28 oC) = 320

Density (g/cm3) = 0.99624

Activity of water = 1.000

Ionic strength = 4.714e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.924e-003

Total CO2 (mol/kg) = 2.924e-003

Temperature (deg C) = 28.700

Electrical balance (eq) = -4.035e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.66

Iterations = 8

Total H = 1.110153e+002

Total O = 5.551601e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 12.0337 0.7207

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.833e-006 2.628e-006 -5.548 -5.580 -0.033

H+ 5.361e-009 5.012e-009 -8.271 -8.300 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.924e-003

HCO3- 2.776e-003 2.583e-003 -2.557 -2.588 -0.031

CaCO3 3.574e-005 3.577e-005 -4.447 -4.446 0.000

CO3-2 3.463e-005 2.594e-005 -4.460 -4.586 -0.125

CaHCO3+ 2.830e-005 2.633e-005 -4.548 -4.580 -0.031

CO2 2.788e-005 2.791e-005 -4.555 -4.554 0.000

MgHCO3+ 1.218e-005 1.131e-005 -4.914 -4.947 -0.032

MgCO3 9.621e-006 9.632e-006 -5.017 -5.016 0.000

NaHCO3 1.346e-008 1.347e-008 -7.871 -7.871 0.000

NaCO3- 5.803e-009 5.389e-009 -8.236 -8.269 -0.032

Ca 1.089e-003

Ca+2 1.013e-003 7.585e-004 -2.994 -3.120 -0.126

CaCO3 3.574e-005 3.577e-005 -4.447 -4.446 0.000

CaHCO3+ 2.830e-005 2.633e-005 -4.548 -4.580 -0.031

CaSO4 1.135e-005 1.136e-005 -4.945 -4.944 0.000

CaOH+ 2.705e-008 2.512e-008 -7.568 -7.600 -0.032

CaHSO4+ 3.770e-013 3.500e-013 -12.424 -12.456 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 3.426e-028

H2 1.713e-028 1.715e-028 -27.766 -27.766 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.805e-009 1.676e-009 -8.744 -8.776 -0.032

KOH 2.131e-012 2.133e-012 -11.671 -11.671 0.000

Mg 5.184e-004

Mg+2 4.893e-004 3.676e-004 -3.310 -3.435 -0.124

MgHCO3+ 1.218e-005 1.131e-005 -4.914 -4.947 -0.032

MgCO3 9.621e-006 9.632e-006 -5.017 -5.016 0.000

MgSO4 6.863e-006 6.870e-006 -5.163 -5.163 0.000

MgOH+ 3.989e-007 3.704e-007 -6.399 -6.431 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.346e-008 1.347e-008 -7.871 -7.871 0.000

NaCO3- 5.803e-009 5.389e-009 -8.236 -8.269 -0.032

NaSO4- 3.719e-009 3.453e-009 -8.430 -8.462 -0.032

NaOH 1.221e-011 1.223e-011 -10.913 -10.913 0.000

O(0) 5.839e-004

O2 2.920e-004 2.923e-004 -3.535 -3.534 0.000

S(6) 1.154e-004

SO4-2 9.715e-005 7.257e-005 -4.013 -4.139 -0.127

CaSO4 1.135e-005 1.136e-005 -4.945 -4.944 0.000

MgSO4 6.863e-006 6.870e-006 -5.163 -5.163 0.000

NaSO4- 3.719e-009 3.453e-009 -8.430 -8.462 -0.032

KSO4- 1.805e-009 1.676e-009 -8.744 -8.776 -0.032

HSO4- 4.134e-011 3.838e-011 -10.384 -10.416 -0.032

CaHSO4+ 3.770e-013 3.500e-013 -12.424 -12.456 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.65 -7.71 -8.36 CaCO3

Calcite 0.80 -7.71 -8.50 CaCO3

CO2(g) -3.04 -4.55 -1.51 CO2

Dolomite 1.45 -15.73 -17.17 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.60 -27.77 -3.17 H2

H2O(g) -1.42 -0.00 1.42 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.62 -3.53 -2.92 O2

Initial solution 101. 30/8/2012 12:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.980e-003 2.980e-003

Ca 1.089e-003 1.089e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.214e-004 6.214e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.330

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 322

Density (g/cm3) = 0.99616

Activity of water = 1.000

Ionic strength = 4.706e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.916e-003

Total CO2 (mol/kg) = 2.916e-003

Temperature (deg C) = 29.000

Electrical balance (eq) = -4.035e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.66

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551603e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9862 0.7186

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.103e-006 2.878e-006 -5.508 -5.541 -0.033

H+ 5.003e-009 4.677e-009 -8.301 -8.330 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.916e-003

HCO3- 2.764e-003 2.571e-003 -2.558 -2.590 -0.031

CaCO3 3.849e-005 3.854e-005 -4.415 -4.414 0.000

CO3-2 3.715e-005 2.783e-005 -4.430 -4.555 -0.125

CaHCO3+ 2.821e-005 2.625e-005 -4.550 -4.581 -0.031

CO2 2.583e-005 2.586e-005 -4.588 -4.587 0.000

MgHCO3+ 1.212e-005 1.126e-005 -4.916 -4.949 -0.032

MgCO3 1.035e-005 1.036e-005 -4.985 -4.984 0.000

NaHCO3 1.340e-008 1.341e-008 -7.873 -7.872 0.000

NaCO3- 6.317e-009 5.866e-009 -8.199 -8.232 -0.032

Ca 1.089e-003

Ca+2 1.011e-003 7.566e-004 -2.995 -3.121 -0.126

CaCO3 3.849e-005 3.854e-005 -4.415 -4.414 0.000

CaHCO3+ 2.821e-005 2.625e-005 -4.550 -4.581 -0.031

CaSO4 1.135e-005 1.136e-005 -4.945 -4.945 0.000

CaOH+ 2.891e-008 2.684e-008 -7.539 -7.571 -0.032

CaHSO4+ 3.532e-013 3.279e-013 -12.452 -12.484 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 2.975e-028

H2 1.488e-028 1.489e-028 -27.828 -27.827 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.814e-009 1.684e-009 -8.741 -8.774 -0.032

KOH 2.283e-012 2.286e-012 -11.641 -11.641 0.000

Mg 5.184e-004

Mg+2 4.886e-004 3.670e-004 -3.311 -3.435 -0.124

MgHCO3+ 1.212e-005 1.126e-005 -4.916 -4.949 -0.032

MgCO3 1.035e-005 1.036e-005 -4.985 -4.984 0.000

MgSO4 6.902e-006 6.910e-006 -5.161 -5.161 0.000

MgOH+ 4.382e-007 4.069e-007 -6.358 -6.391 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.340e-008 1.341e-008 -7.873 -7.872 0.000

NaCO3- 6.317e-009 5.866e-009 -8.199 -8.232 -0.032

NaSO4- 3.724e-009 3.458e-009 -8.429 -8.461 -0.032

NaOH 1.309e-011 1.310e-011 -10.883 -10.883 0.000

O(0) 6.214e-004

O2 3.107e-004 3.110e-004 -3.508 -3.507 0.000

S(6) 1.154e-004

SO4-2 9.711e-005 7.255e-005 -4.013 -4.139 -0.127

CaSO4 1.135e-005 1.136e-005 -4.945 -4.945 0.000

MgSO4 6.902e-006 6.910e-006 -5.161 -5.161 0.000

NaSO4- 3.724e-009 3.458e-009 -8.429 -8.461 -0.032

KSO4- 1.814e-009 1.684e-009 -8.741 -8.774 -0.032

HSO4- 3.882e-011 3.605e-011 -10.411 -10.443 -0.032

CaHSO4+ 3.532e-013 3.279e-013 -12.452 -12.484 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.69 -7.68 -8.36 CaCO3

Calcite 0.83 -7.68 -8.50 CaCO3

CO2(g) -3.07 -4.59 -1.51 CO2

Dolomite 1.51 -15.67 -17.18 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.66 -27.83 -3.17 H2

H2O(g) -1.41 -0.00 1.41 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.59 -3.51 -2.92 O2

Initial solution 102. 30/8/2012 13:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.938e-003 2.938e-003

Ca 1.074e-003 1.074e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.408e-004 6.408e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.310

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 321

Density (g/cm3) = 0.99607

Activity of water = 1.000

Ionic strength = 4.662e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.880e-003

Total CO2 (mol/kg) = 2.880e-003

Temperature (deg C) = 29.300

Electrical balance (eq) = -2.899e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.48

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551594e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9854 0.7192

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.027e-006 2.809e-006 -5.519 -5.551 -0.032

H+ 5.238e-009 4.898e-009 -8.281 -8.310 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.880e-003

HCO3- 2.732e-003 2.542e-003 -2.564 -2.595 -0.031

CaCO3 3.639e-005 3.643e-005 -4.439 -4.439 0.000

CO3-2 3.523e-005 2.642e-005 -4.453 -4.578 -0.125

CaHCO3+ 2.769e-005 2.577e-005 -4.558 -4.589 -0.031

CO2 2.666e-005 2.669e-005 -4.574 -4.574 0.000

MgHCO3+ 1.203e-005 1.117e-005 -4.920 -4.952 -0.032

MgCO3 9.895e-006 9.905e-006 -5.005 -5.004 0.000

NaHCO3 1.325e-008 1.327e-008 -7.878 -7.877 0.000

NaCO3- 6.087e-009 5.654e-009 -8.216 -8.248 -0.032

Ca 1.074e-003

Ca+2 9.983e-004 7.482e-004 -3.001 -3.126 -0.125

CaCO3 3.639e-005 3.643e-005 -4.439 -4.439 0.000

CaHCO3+ 2.769e-005 2.577e-005 -4.558 -4.589 -0.031

CaSO4 1.127e-005 1.128e-005 -4.948 -4.948 0.000

CaOH+ 2.729e-008 2.535e-008 -7.564 -7.596 -0.032

CaHSO4+ 3.685e-013 3.423e-013 -12.434 -12.466 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.274 -0.032

H(0) 3.253e-028

H2 1.626e-028 1.628e-028 -27.789 -27.788 0.000

K 3.325e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.825e-009 1.695e-009 -8.739 -8.771 -0.032

KOH 2.181e-012 2.184e-012 -11.661 -11.661 0.000

Mg 5.184e-004

Mg+2 4.891e-004 3.678e-004 -3.311 -3.434 -0.124

MgHCO3+ 1.203e-005 1.117e-005 -4.920 -4.952 -0.032

MgCO3 9.895e-006 9.905e-006 -5.005 -5.004 0.000

MgSO4 6.976e-006 6.984e-006 -5.156 -5.156 0.000

MgOH+ 4.304e-007 3.997e-007 -6.366 -6.398 -0.032

Na 1.001e-005

Na+ 9.984e-006 9.279e-006 -5.001 -5.032 -0.032

NaHCO3 1.325e-008 1.327e-008 -7.878 -7.877 0.000

NaCO3- 6.087e-009 5.654e-009 -8.216 -8.248 -0.032

NaSO4- 3.736e-009 3.470e-009 -8.428 -8.460 -0.032

NaOH 1.250e-011 1.252e-011 -10.903 -10.903 0.000

O(0) 6.408e-004

O2 3.204e-004 3.207e-004 -3.494 -3.494 0.000

S(6) 1.154e-004

SO4-2 9.712e-005 7.263e-005 -4.013 -4.139 -0.126

CaSO4 1.127e-005 1.128e-005 -4.948 -4.948 0.000

MgSO4 6.976e-006 6.984e-006 -5.156 -5.156 0.000

NaSO4- 3.736e-009 3.470e-009 -8.428 -8.460 -0.032

KSO4- 1.825e-009 1.695e-009 -8.739 -8.771 -0.032

HSO4- 4.097e-011 3.805e-011 -10.388 -10.420 -0.032

CaHSO4+ 3.685e-013 3.423e-013 -12.434 -12.466 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.66 -7.70 -8.36 CaCO3

Calcite 0.80 -7.70 -8.51 CaCO3

CO2(g) -3.06 -4.57 -1.52 CO2

Dolomite 1.47 -15.72 -17.19 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.62 -27.79 -3.17 H2

H2O(g) -1.40 -0.00 1.40 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.57 -3.49 -2.92 O2

Initial solution 103. 30/8/2012 13:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.980e-003 2.980e-003

Ca 1.089e-003 1.089e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.652e-004 6.652e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.340

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 326

Density (g/cm3) = 0.99595

Activity of water = 1.000

Ionic strength = 4.699e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.911e-003

Total CO2 (mol/kg) = 2.911e-003

Temperature (deg C) = 29.700

Electrical balance (eq) = -4.035e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.66

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551606e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9273 0.7167

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.340e-006 3.098e-006 -5.476 -5.509 -0.033

H+ 4.889e-009 4.571e-009 -8.311 -8.340 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.911e-003

HCO3- 2.756e-003 2.564e-003 -2.560 -2.591 -0.031

CaCO3 4.034e-005 4.038e-005 -4.394 -4.394 0.000

CO3-2 3.840e-005 2.876e-005 -4.416 -4.541 -0.126

CaHCO3+ 2.833e-005 2.635e-005 -4.548 -4.579 -0.031

CO2 2.500e-005 2.503e-005 -4.602 -4.602 0.000

MgHCO3+ 1.212e-005 1.125e-005 -4.916 -4.949 -0.032

MgCO3 1.080e-005 1.081e-005 -4.967 -4.966 0.000

NaHCO3 1.336e-008 1.337e-008 -7.874 -7.874 0.000

NaCO3- 6.756e-009 6.273e-009 -8.170 -8.203 -0.032

Ca 1.089e-003

Ca+2 1.009e-003 7.550e-004 -2.996 -3.122 -0.126

CaCO3 4.034e-005 4.038e-005 -4.394 -4.394 0.000

CaHCO3+ 2.833e-005 2.635e-005 -4.548 -4.579 -0.031

CaSO4 1.138e-005 1.139e-005 -4.944 -4.943 0.000

CaOH+ 2.952e-008 2.741e-008 -7.530 -7.562 -0.032

CaHSO4+ 3.493e-013 3.244e-013 -12.457 -12.489 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 2.822e-028

H2 1.411e-028 1.413e-028 -27.850 -27.850 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.832e-009 1.701e-009 -8.737 -8.769 -0.032

KOH 2.336e-012 2.339e-012 -11.631 -11.631 0.000

Mg 5.184e-004

Mg+2 4.880e-004 3.665e-004 -3.312 -3.436 -0.124

MgHCO3+ 1.212e-005 1.125e-005 -4.916 -4.949 -0.032

MgCO3 1.080e-005 1.081e-005 -4.967 -4.966 0.000

MgSO4 7.004e-006 7.011e-006 -5.155 -5.154 0.000

MgOH+ 4.761e-007 4.421e-007 -6.322 -6.354 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.275e-006 -5.001 -5.033 -0.032

NaHCO3 1.336e-008 1.337e-008 -7.874 -7.874 0.000

NaCO3- 6.756e-009 6.273e-009 -8.170 -8.203 -0.032

NaSO4- 3.735e-009 3.468e-009 -8.428 -8.460 -0.032

NaOH 1.339e-011 1.341e-011 -10.873 -10.873 0.000

O(0) 6.652e-004

O2 3.326e-004 3.329e-004 -3.478 -3.478 0.000

S(6) 1.154e-004

SO4-2 9.698e-005 7.244e-005 -4.013 -4.140 -0.127

CaSO4 1.138e-005 1.139e-005 -4.944 -4.943 0.000

MgSO4 7.004e-006 7.011e-006 -5.155 -5.154 0.000

NaSO4- 3.735e-009 3.468e-009 -8.428 -8.460 -0.032

KSO4- 1.832e-009 1.701e-009 -8.737 -8.769 -0.032

HSO4- 3.849e-011 3.574e-011 -10.415 -10.447 -0.032

CaHSO4+ 3.493e-013 3.244e-013 -12.457 -12.489 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.38 CaSO4

Aragonite 0.70 -7.66 -8.37 CaCO3

Calcite 0.84 -7.66 -8.51 CaCO3

CO2(g) -3.08 -4.60 -1.52 CO2

Dolomite 1.56 -15.64 -17.20 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.68 -27.85 -3.17 H2

H2O(g) -1.39 -0.00 1.39 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.55 -3.48 -2.92 O2

Initial solution 104. 30/8/2012 13:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.938e-003 2.938e-003

Ca 1.074e-003 1.074e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.645e-004 6.645e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.350

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 324

Density (g/cm3) = 0.99592

Activity of water = 1.000

Ionic strength = 4.651e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.868e-003

Total CO2 (mol/kg) = 2.868e-003

Temperature (deg C) = 29.800

Electrical balance (eq) = -2.899e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.48

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551593e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.9092 0.7158

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.441e-006 3.193e-006 -5.463 -5.496 -0.032

H+ 4.777e-009 4.467e-009 -8.321 -8.350 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.868e-003

HCO3- 2.715e-003 2.526e-003 -2.566 -2.597 -0.031

CaCO3 4.032e-005 4.036e-005 -4.395 -4.394 0.000

CO3-2 3.873e-005 2.905e-005 -4.412 -4.537 -0.125

CaHCO3+ 2.758e-005 2.567e-005 -4.559 -4.591 -0.031

CO2 2.405e-005 2.407e-005 -4.619 -4.618 0.000

MgHCO3+ 1.196e-005 1.111e-005 -4.922 -4.954 -0.032

MgCO3 1.094e-005 1.095e-005 -4.961 -4.961 0.000

NaHCO3 1.317e-008 1.318e-008 -7.880 -7.880 0.000

NaCO3- 6.857e-009 6.369e-009 -8.164 -8.196 -0.032

Ca 1.074e-003

Ca+2 9.944e-004 7.454e-004 -3.002 -3.128 -0.125

CaCO3 4.032e-005 4.036e-005 -4.395 -4.394 0.000

CaHCO3+ 2.758e-005 2.567e-005 -4.559 -4.591 -0.031

CaSO4 1.127e-005 1.128e-005 -4.948 -4.948 0.000

CaOH+ 2.981e-008 2.769e-008 -7.526 -7.558 -0.032

CaHSO4+ 3.384e-013 3.143e-013 -12.471 -12.503 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.316e-005 -4.242 -4.274 -0.032

H(0) 2.692e-028

H2 1.346e-028 1.348e-028 -27.871 -27.870 0.000

K 3.325e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.839e-009 1.708e-009 -8.735 -8.767 -0.032

KOH 2.392e-012 2.394e-012 -11.621 -11.621 0.000

Mg 5.184e-004

Mg+2 4.880e-004 3.670e-004 -3.312 -3.435 -0.124

MgHCO3+ 1.196e-005 1.111e-005 -4.922 -4.954 -0.032

MgCO3 1.094e-005 1.095e-005 -4.961 -4.961 0.000

MgSO4 7.044e-006 7.052e-006 -5.152 -5.152 0.000

MgOH+ 4.919e-007 4.569e-007 -6.308 -6.340 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.279e-006 -5.001 -5.033 -0.032

NaHCO3 1.317e-008 1.318e-008 -7.880 -7.880 0.000

NaCO3- 6.857e-009 6.369e-009 -8.164 -8.196 -0.032

NaSO4- 3.745e-009 3.478e-009 -8.427 -8.459 -0.032

NaOH 1.371e-011 1.372e-011 -10.863 -10.863 0.000

O(0) 6.645e-004

O2 3.323e-004 3.326e-004 -3.479 -3.478 0.000

S(6) 1.154e-004

SO4-2 9.705e-005 7.258e-005 -4.013 -4.139 -0.126

CaSO4 1.127e-005 1.128e-005 -4.948 -4.948 0.000

MgSO4 7.044e-006 7.052e-006 -5.152 -5.152 0.000

NaSO4- 3.745e-009 3.478e-009 -8.427 -8.459 -0.032

KSO4- 1.839e-009 1.708e-009 -8.735 -8.767 -0.032

HSO4- 3.776e-011 3.507e-011 -10.423 -10.455 -0.032

CaHSO4+ 3.384e-013 3.143e-013 -12.471 -12.503 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.38 CaSO4

Aragonite 0.70 -7.66 -8.37 CaCO3

Calcite 0.84 -7.66 -8.51 CaCO3

CO2(g) -3.10 -4.62 -1.52 CO2

Dolomite 1.56 -15.64 -17.20 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.70 -27.87 -3.17 H2

H2O(g) -1.39 -0.00 1.39 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.55 -3.48 -2.93 O2

Initial solution 105. 30/8/2012 13:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.802e-004 5.802e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.340

pe = 4.000

Specific Conductance (uS/cm, 29 oC) = 326

Density (g/cm3) = 0.99589

Activity of water = 1.000

Ionic strength = 4.675e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.891e-003

Total CO2 (mol/kg) = 2.891e-003

Temperature (deg C) = 29.900

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551591e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8964 0.7153

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.388e-006 3.143e-006 -5.470 -5.503 -0.033

H+ 4.889e-009 4.571e-009 -8.311 -8.340 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.891e-003

HCO3- 2.737e-003 2.546e-003 -2.563 -2.594 -0.031

CaCO3 4.013e-005 4.017e-005 -4.397 -4.396 0.000

CO3-2 3.824e-005 2.866e-005 -4.417 -4.543 -0.125

CaHCO3+ 2.802e-005 2.607e-005 -4.553 -4.584 -0.031

CO2 2.478e-005 2.480e-005 -4.606 -4.605 0.000

MgHCO3+ 1.205e-005 1.119e-005 -4.919 -4.951 -0.032

MgCO3 1.080e-005 1.081e-005 -4.966 -4.966 0.000

NaHCO3 1.327e-008 1.328e-008 -7.877 -7.877 0.000

NaCO3- 6.799e-009 6.314e-009 -8.168 -8.200 -0.032

Ca 1.081e-003

Ca+2 1.002e-003 7.502e-004 -2.999 -3.125 -0.126

CaCO3 4.013e-005 4.017e-005 -4.397 -4.396 0.000

CaHCO3+ 2.802e-005 2.607e-005 -4.553 -4.584 -0.031

CaSO4 1.134e-005 1.135e-005 -4.946 -4.945 0.000

CaOH+ 2.933e-008 2.724e-008 -7.533 -7.565 -0.032

CaHSO4+ 3.489e-013 3.240e-013 -12.457 -12.489 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.275 -0.032

H(0) 2.817e-028

H2 1.408e-028 1.410e-028 -27.851 -27.851 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.840e-009 1.708e-009 -8.735 -8.767 -0.032

KOH 2.337e-012 2.339e-012 -11.631 -11.631 0.000

Mg 5.184e-004

Mg+2 4.880e-004 3.667e-004 -3.312 -3.436 -0.124

MgHCO3+ 1.205e-005 1.119e-005 -4.919 -4.951 -0.032

MgCO3 1.080e-005 1.081e-005 -4.966 -4.966 0.000

MgSO4 7.047e-006 7.055e-006 -5.152 -5.152 0.000

MgOH+ 4.847e-007 4.502e-007 -6.314 -6.347 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.327e-008 1.328e-008 -7.877 -7.877 0.000

NaCO3- 6.799e-009 6.314e-009 -8.168 -8.200 -0.032

NaSO4- 3.741e-009 3.474e-009 -8.427 -8.459 -0.032

NaOH 1.339e-011 1.341e-011 -10.873 -10.873 0.000

O(0) 5.802e-004

O2 2.901e-004 2.904e-004 -3.537 -3.537 0.000

S(6) 1.154e-004

SO4-2 9.698e-005 7.248e-005 -4.013 -4.140 -0.126

CaSO4 1.134e-005 1.135e-005 -4.946 -4.945 0.000

MgSO4 7.047e-006 7.055e-006 -5.152 -5.152 0.000

NaSO4- 3.741e-009 3.474e-009 -8.427 -8.459 -0.032

KSO4- 1.840e-009 1.708e-009 -8.735 -8.767 -0.032

HSO4- 3.868e-011 3.592e-011 -10.413 -10.445 -0.032

CaHSO4+ 3.489e-013 3.240e-013 -12.457 -12.489 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.39 CaSO4

Aragonite 0.70 -7.67 -8.37 CaCO3

Calcite 0.84 -7.67 -8.51 CaCO3

CO2(g) -3.08 -4.61 -1.52 CO2

Dolomite 1.56 -15.65 -17.20 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.68 -27.85 -3.17 H2

H2O(g) -1.39 -0.00 1.39 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.61 -3.54 -2.93 O2

Initial solution 106. 30/8/2012 14:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.990e-003 2.990e-003

Ca 1.092e-003 1.092e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.608e-004 6.608e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.380

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 329

Density (g/cm3) = 0.99583

Activity of water = 1.000

Ionic strength = 4.699e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.910e-003

Total CO2 (mol/kg) = 2.910e-003

Temperature (deg C) = 30.100

Electrical balance (eq) = -4.336e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.71

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551605e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8545 0.7133

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.769e-006 3.496e-006 -5.424 -5.456 -0.033

H+ 4.459e-009 4.169e-009 -8.351 -8.380 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.910e-003

HCO3- 2.747e-003 2.556e-003 -2.561 -2.592 -0.031

CaCO3 4.477e-005 4.482e-005 -4.349 -4.349 0.000

CO3-2 4.227e-005 3.165e-005 -4.374 -4.500 -0.126

CaHCO3+ 2.835e-005 2.637e-005 -4.547 -4.579 -0.031

CO2 2.264e-005 2.266e-005 -4.645 -4.645 0.000

MgHCO3+ 1.208e-005 1.121e-005 -4.918 -4.950 -0.032

MgCO3 1.193e-005 1.194e-005 -4.923 -4.923 0.000

NaHCO3 1.331e-008 1.333e-008 -7.876 -7.875 0.000

NaCO3- 7.582e-009 7.039e-009 -8.120 -8.152 -0.032

Ca 1.092e-003

Ca+2 1.008e-003 7.543e-004 -2.997 -3.122 -0.126

CaCO3 4.477e-005 4.482e-005 -4.349 -4.349 0.000

CaHCO3+ 2.835e-005 2.637e-005 -4.547 -4.579 -0.031

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

CaOH+ 3.234e-008 3.003e-008 -7.490 -7.523 -0.032

CaHSO4+ 3.209e-013 2.980e-013 -12.494 -12.526 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 2.338e-028

H2 1.169e-028 1.170e-028 -27.932 -27.932 0.000

K 3.326e-006

K+ 3.324e-006 3.083e-006 -5.478 -5.511 -0.033

KSO4- 1.843e-009 1.711e-009 -8.734 -8.767 -0.032

KOH 2.562e-012 2.565e-012 -11.591 -11.591 0.000

Mg 5.184e-004

Mg+2 4.868e-004 3.656e-004 -3.313 -3.437 -0.124

MgHCO3+ 1.208e-005 1.121e-005 -4.918 -4.950 -0.032

MgCO3 1.193e-005 1.194e-005 -4.923 -4.923 0.000

MgSO4 7.049e-006 7.057e-006 -5.152 -5.151 0.000

MgOH+ 5.393e-007 5.007e-007 -6.268 -6.300 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.274e-006 -5.001 -5.033 -0.032

NaHCO3 1.331e-008 1.333e-008 -7.876 -7.875 0.000

NaCO3- 7.582e-009 7.039e-009 -8.120 -8.152 -0.032

NaSO4- 3.740e-009 3.473e-009 -8.427 -8.459 -0.032

NaOH 1.468e-011 1.470e-011 -10.833 -10.833 0.000

O(0) 6.608e-004

O2 3.304e-004 3.308e-004 -3.481 -3.480 0.000

S(6) 1.154e-004

SO4-2 9.691e-005 7.237e-005 -4.014 -4.140 -0.127

CaSO4 1.140e-005 1.141e-005 -4.943 -4.943 0.000

MgSO4 7.049e-006 7.057e-006 -5.152 -5.151 0.000

NaSO4- 3.740e-009 3.473e-009 -8.427 -8.459 -0.032

KSO4- 1.843e-009 1.711e-009 -8.734 -8.767 -0.032

HSO4- 3.539e-011 3.286e-011 -10.451 -10.483 -0.032

CaHSO4+ 3.209e-013 2.980e-013 -12.494 -12.526 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.26 -4.39 CaSO4

Aragonite 0.75 -7.62 -8.37 CaCO3

Calcite 0.89 -7.62 -8.51 CaCO3

CO2(g) -3.12 -4.64 -1.53 CO2

Dolomite 1.65 -15.56 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.26 -4.58 CaSO4:2H2O

H2(g) -24.76 -27.93 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.55 -3.48 -2.93 O2

Initial solution 107. 30/8/2012 14:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.897e-003 2.897e-003

Ca 1.059e-003 1.059e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.402e-004 6.402e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.390

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 322

Density (g/cm3) = 0.99579

Activity of water = 1.000

Ionic strength = 4.594e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.817e-003

Total CO2 (mol/kg) = 2.817e-003

Temperature (deg C) = 30.200

Electrical balance (eq) = -1.779e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.30

Iterations = 8

Total H = 1.110151e+002

Total O = 5.551575e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8330 0.7122

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.882e-006 3.603e-006 -5.411 -5.443 -0.032

H+ 4.355e-009 4.074e-009 -8.361 -8.390 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.817e-003

HCO3- 2.660e-003 2.476e-003 -2.575 -2.606 -0.031

CaCO3 4.335e-005 4.339e-005 -4.363 -4.363 0.000

CO3-2 4.186e-005 3.144e-005 -4.378 -4.503 -0.124

CaHCO3+ 2.673e-005 2.488e-005 -4.573 -4.604 -0.031

CO2 2.141e-005 2.144e-005 -4.669 -4.669 0.000

MgCO3 1.191e-005 1.192e-005 -4.924 -4.924 0.000

MgHCO3+ 1.174e-005 1.091e-005 -4.930 -4.962 -0.032

NaHCO3 1.291e-008 1.292e-008 -7.889 -7.889 0.000

NaCO3- 7.567e-009 7.031e-009 -8.121 -8.153 -0.032

Ca 1.059e-003

Ca+2 9.774e-004 7.336e-004 -3.010 -3.135 -0.125

CaCO3 4.335e-005 4.339e-005 -4.363 -4.363 0.000

CaHCO3+ 2.673e-005 2.488e-005 -4.573 -4.604 -0.031

CaSO4 1.115e-005 1.116e-005 -4.953 -4.952 0.000

CaOH+ 3.216e-008 2.988e-008 -7.493 -7.525 -0.032

CaHSO4+ 3.070e-013 2.852e-013 -12.513 -12.545 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.318e-005 -4.242 -4.274 -0.032

H(0) 2.231e-028

H2 1.115e-028 1.117e-028 -27.953 -27.952 0.000

K 3.325e-006

K+ 3.324e-006 3.086e-006 -5.478 -5.511 -0.032

KSO4- 1.855e-009 1.724e-009 -8.732 -8.764 -0.032

KOH 2.623e-012 2.626e-012 -11.581 -11.581 0.000

Mg 5.184e-004

Mg+2 4.871e-004 3.668e-004 -3.312 -3.436 -0.123

MgCO3 1.191e-005 1.192e-005 -4.924 -4.924 0.000

MgHCO3+ 1.174e-005 1.091e-005 -4.930 -4.962 -0.032

MgSO4 7.124e-006 7.132e-006 -5.147 -5.147 0.000

MgOH+ 5.581e-007 5.186e-007 -6.253 -6.285 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.281e-006 -5.001 -5.032 -0.032

NaHCO3 1.291e-008 1.292e-008 -7.889 -7.889 0.000

NaCO3- 7.567e-009 7.031e-009 -8.121 -8.153 -0.032

NaSO4- 3.760e-009 3.494e-009 -8.425 -8.457 -0.032

NaOH 1.504e-011 1.505e-011 -10.823 -10.822 0.000

O(0) 6.402e-004

O2 3.201e-004 3.204e-004 -3.495 -3.494 0.000

S(6) 1.154e-004

SO4-2 9.709e-005 7.271e-005 -4.013 -4.138 -0.126

CaSO4 1.115e-005 1.116e-005 -4.953 -4.952 0.000

MgSO4 7.124e-006 7.132e-006 -5.147 -5.147 0.000

NaSO4- 3.760e-009 3.494e-009 -8.425 -8.457 -0.032

KSO4- 1.855e-009 1.724e-009 -8.732 -8.764 -0.032

HSO4- 3.480e-011 3.234e-011 -10.458 -10.490 -0.032

CaHSO4+ 3.070e-013 2.852e-013 -12.513 -12.545 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.89 -7.27 -4.39 CaSO4

Aragonite 0.73 -7.64 -8.37 CaCO3

Calcite 0.87 -7.64 -8.51 CaCO3

CO2(g) -3.14 -4.67 -1.53 CO2

Dolomite 1.63 -15.58 -17.21 CaMg(CO3)2

Gypsum -2.69 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.78 -27.95 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.57 -3.49 -2.93 O2

Initial solution 108. 30/8/2012 14:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.928e-003 2.928e-003

Ca 1.070e-003 1.070e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 7.164e-004 7.164e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.380

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 326

Density (g/cm3) = 0.99574

Activity of water = 1.000

Ionic strength = 4.629e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.849e-003

Total CO2 (mol/kg) = 2.849e-003

Temperature (deg C) = 30.400

Electrical balance (eq) = -2.631e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.44

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551592e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8393 0.7130

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.849e-006 3.572e-006 -5.415 -5.447 -0.032

H+ 4.458e-009 4.169e-009 -8.351 -8.380 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.849e-003

HCO3- 2.691e-003 2.504e-003 -2.570 -2.601 -0.031

CaCO3 4.359e-005 4.364e-005 -4.361 -4.360 0.000

CO3-2 4.155e-005 3.117e-005 -4.381 -4.506 -0.125

CaHCO3+ 2.736e-005 2.546e-005 -4.563 -4.594 -0.031

CO2 2.212e-005 2.214e-005 -4.655 -4.655 0.000

MgHCO3+ 1.187e-005 1.103e-005 -4.926 -4.958 -0.032

MgCO3 1.183e-005 1.184e-005 -4.927 -4.927 0.000

NaHCO3 1.305e-008 1.307e-008 -7.884 -7.884 0.000

NaCO3- 7.577e-009 7.038e-009 -8.120 -8.153 -0.032

Ca 1.070e-003

Ca+2 9.877e-004 7.405e-004 -3.005 -3.130 -0.125

CaCO3 4.359e-005 4.364e-005 -4.361 -4.360 0.000

CaHCO3+ 2.736e-005 2.546e-005 -4.563 -4.594 -0.031

CaSO4 1.125e-005 1.126e-005 -4.949 -4.948 0.000

CaOH+ 3.174e-008 2.948e-008 -7.498 -7.530 -0.032

CaHSO4+ 3.179e-013 2.953e-013 -12.498 -12.530 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.316e-005 -4.242 -4.274 -0.032

H(0) 2.331e-028

H2 1.166e-028 1.167e-028 -27.933 -27.933 0.000

K 3.325e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.857e-009 1.725e-009 -8.731 -8.763 -0.032

KOH 2.563e-012 2.566e-012 -11.591 -11.591 0.000

Mg 5.184e-004

Mg+2 4.870e-004 3.663e-004 -3.312 -3.436 -0.124

MgHCO3+ 1.187e-005 1.103e-005 -4.926 -4.958 -0.032

MgCO3 1.183e-005 1.184e-005 -4.927 -4.927 0.000

MgSO4 7.135e-006 7.143e-006 -5.147 -5.146 0.000

MgOH+ 5.545e-007 5.151e-007 -6.256 -6.288 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.279e-006 -5.001 -5.033 -0.032

NaHCO3 1.305e-008 1.307e-008 -7.884 -7.884 0.000

NaCO3- 7.577e-009 7.038e-009 -8.120 -8.153 -0.032

NaSO4- 3.756e-009 3.489e-009 -8.425 -8.457 -0.032

NaOH 1.469e-011 1.470e-011 -10.833 -10.833 0.000

O(0) 7.164e-004

O2 3.582e-004 3.586e-004 -3.446 -3.445 0.000

S(6) 1.154e-004

SO4-2 9.698e-005 7.255e-005 -4.013 -4.139 -0.126

CaSO4 1.125e-005 1.126e-005 -4.949 -4.948 0.000

MgSO4 7.135e-006 7.143e-006 -5.147 -5.146 0.000

NaSO4- 3.756e-009 3.489e-009 -8.425 -8.457 -0.032

KSO4- 1.857e-009 1.725e-009 -8.731 -8.763 -0.032

HSO4- 3.571e-011 3.317e-011 -10.447 -10.479 -0.032

CaHSO4+ 3.179e-013 2.953e-013 -12.498 -12.530 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.74 -7.64 -8.37 CaCO3

Calcite 0.88 -7.64 -8.51 CaCO3

CO2(g) -3.13 -4.65 -1.53 CO2

Dolomite 1.63 -15.58 -17.21 CaMg(CO3)2

Gypsum -2.69 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.76 -27.93 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.52 -3.45 -2.93 O2

Initial solution 109. 30/8/2012 15:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.214e-004 6.214e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.390

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 329

Density (g/cm3) = 0.99571

Activity of water = 1.000

Ionic strength = 4.660e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.876e-003

Total CO2 (mol/kg) = 2.876e-003

Temperature (deg C) = 30.500

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551591e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8058 0.7113

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.968e-006 3.682e-006 -5.401 -5.434 -0.033

H+ 4.357e-009 4.074e-009 -8.361 -8.390 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.876e-003

HCO3- 2.713e-003 2.525e-003 -2.566 -2.598 -0.031

CaCO3 4.552e-005 4.557e-005 -4.342 -4.341 0.000

CO3-2 4.299e-005 3.222e-005 -4.367 -4.492 -0.125

CaHCO3+ 2.784e-005 2.590e-005 -4.555 -4.587 -0.031

CO2 2.177e-005 2.179e-005 -4.662 -4.662 0.000

MgCO3 1.222e-005 1.223e-005 -4.913 -4.912 0.000

MgHCO3+ 1.196e-005 1.110e-005 -4.922 -4.955 -0.032

NaHCO3 1.316e-008 1.317e-008 -7.881 -7.880 0.000

NaCO3- 7.869e-009 7.308e-009 -8.104 -8.136 -0.032

Ca 1.081e-003

Ca+2 9.964e-004 7.464e-004 -3.002 -3.127 -0.125

CaCO3 4.552e-005 4.557e-005 -4.342 -4.341 0.000

CaHCO3+ 2.784e-005 2.590e-005 -4.555 -4.587 -0.031

CaSO4 1.133e-005 1.134e-005 -4.946 -4.945 0.000

CaOH+ 3.274e-008 3.040e-008 -7.485 -7.517 -0.032

CaHSO4+ 3.134e-013 2.910e-013 -12.504 -12.536 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.275 -0.032

H(0) 2.224e-028

H2 1.112e-028 1.113e-028 -27.954 -27.953 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.857e-009 1.725e-009 -8.731 -8.763 -0.032

KOH 2.622e-012 2.625e-012 -11.581 -11.581 0.000

Mg 5.184e-004

Mg+2 4.865e-004 3.657e-004 -3.313 -3.437 -0.124

MgCO3 1.222e-005 1.223e-005 -4.913 -4.912 0.000

MgHCO3+ 1.196e-005 1.110e-005 -4.922 -4.955 -0.032

MgSO4 7.128e-006 7.135e-006 -5.147 -5.147 0.000

MgOH+ 5.714e-007 5.307e-007 -6.243 -6.275 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.316e-008 1.317e-008 -7.881 -7.880 0.000

NaCO3- 7.869e-009 7.308e-009 -8.104 -8.136 -0.032

NaSO4- 3.752e-009 3.485e-009 -8.426 -8.458 -0.032

NaOH 1.503e-011 1.504e-011 -10.823 -10.823 0.000

O(0) 6.214e-004

O2 3.107e-004 3.110e-004 -3.508 -3.507 0.000

S(6) 1.154e-004

SO4-2 9.690e-005 7.243e-005 -4.014 -4.140 -0.126

CaSO4 1.133e-005 1.134e-005 -4.946 -4.945 0.000

MgSO4 7.128e-006 7.135e-006 -5.147 -5.147 0.000

NaSO4- 3.752e-009 3.485e-009 -8.426 -8.458 -0.032

KSO4- 1.857e-009 1.725e-009 -8.731 -8.763 -0.032

HSO4- 3.492e-011 3.243e-011 -10.457 -10.489 -0.032

CaHSO4+ 3.134e-013 2.910e-013 -12.504 -12.536 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.75 -7.62 -8.37 CaCO3

Calcite 0.89 -7.62 -8.51 CaCO3

CO2(g) -3.13 -4.66 -1.53 CO2

Dolomite 1.67 -15.55 -17.22 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.78 -27.95 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.58 -3.51 -2.93 O2

Initial solution 110. 30/8/2012 15:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.949e-003 2.949e-003

Ca 1.077e-003 1.077e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.589e-004 6.589e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.370

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 328

Density (g/cm3) = 0.99574

Activity of water = 1.000

Ionic strength = 4.654e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.871e-003

Total CO2 (mol/kg) = 2.871e-003

Temperature (deg C) = 30.400

Electrical balance (eq) = -3.183e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.52

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551593e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8402 0.7131

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.762e-006 3.491e-006 -5.425 -5.457 -0.033

H+ 4.562e-009 4.266e-009 -8.341 -8.370 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.871e-003

HCO3- 2.713e-003 2.524e-003 -2.567 -2.598 -0.031

CaCO3 4.324e-005 4.328e-005 -4.364 -4.364 0.000

CO3-2 4.097e-005 3.071e-005 -4.388 -4.513 -0.125

CaHCO3+ 2.777e-005 2.584e-005 -4.556 -4.588 -0.031

CO2 2.282e-005 2.284e-005 -4.642 -4.641 0.000

MgHCO3+ 1.196e-005 1.111e-005 -4.922 -4.954 -0.032

MgCO3 1.165e-005 1.166e-005 -4.934 -4.933 0.000

NaHCO3 1.316e-008 1.317e-008 -7.881 -7.880 0.000

NaCO3- 7.465e-009 6.933e-009 -8.127 -8.159 -0.032

Ca 1.077e-003

Ca+2 9.950e-004 7.455e-004 -3.002 -3.128 -0.125

CaCO3 4.324e-005 4.328e-005 -4.364 -4.364 0.000

CaHCO3+ 2.777e-005 2.584e-005 -4.556 -4.588 -0.031

CaSO4 1.131e-005 1.133e-005 -4.946 -4.946 0.000

CaOH+ 3.123e-008 2.900e-008 -7.505 -7.538 -0.032

CaHSO4+ 3.272e-013 3.038e-013 -12.485 -12.517 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.274 -0.032

H(0) 2.441e-028

H2 1.221e-028 1.222e-028 -27.913 -27.913 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.855e-009 1.723e-009 -8.732 -8.764 -0.032

KOH 2.504e-012 2.507e-012 -11.601 -11.601 0.000

Mg 5.184e-004

Mg+2 4.871e-004 3.662e-004 -3.312 -3.436 -0.124

MgHCO3+ 1.196e-005 1.111e-005 -4.922 -4.954 -0.032

MgCO3 1.165e-005 1.166e-005 -4.934 -4.933 0.000

MgSO4 7.123e-006 7.131e-006 -5.147 -5.147 0.000

MgOH+ 5.417e-007 5.031e-007 -6.266 -6.298 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.316e-008 1.317e-008 -7.881 -7.880 0.000

NaCO3- 7.465e-009 6.933e-009 -8.127 -8.159 -0.032

NaSO4- 3.752e-009 3.484e-009 -8.426 -8.458 -0.032

NaOH 1.435e-011 1.437e-011 -10.843 -10.843 0.000

O(0) 6.589e-004

O2 3.295e-004 3.298e-004 -3.482 -3.482 0.000

S(6) 1.154e-004

SO4-2 9.693e-005 7.246e-005 -4.014 -4.140 -0.126

CaSO4 1.131e-005 1.133e-005 -4.946 -4.946 0.000

MgSO4 7.123e-006 7.131e-006 -5.147 -5.147 0.000

NaSO4- 3.752e-009 3.484e-009 -8.426 -8.458 -0.032

KSO4- 1.855e-009 1.723e-009 -8.732 -8.764 -0.032

HSO4- 3.650e-011 3.390e-011 -10.438 -10.470 -0.032

CaHSO4+ 3.272e-013 3.038e-013 -12.485 -12.517 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.73 -7.64 -8.37 CaCO3

Calcite 0.87 -7.64 -8.51 CaCO3

CO2(g) -3.11 -4.64 -1.53 CO2

Dolomite 1.62 -15.59 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.74 -27.91 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.55 -3.48 -2.93 O2

Initial solution 111. 30/8/2012 15:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.928e-003 2.928e-003

Ca 1.070e-003 1.070e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 6.127e-004 6.127e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.390

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 326

Density (g/cm3) = 0.99573

Activity of water = 1.000

Ionic strength = 4.626e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.846e-003

Total CO2 (mol/kg) = 2.846e-003

Temperature (deg C) = 30.400

Electrical balance (eq) = -2.631e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.44

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551581e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8123 0.7114

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.939e-006 3.655e-006 -5.405 -5.437 -0.032

H+ 4.356e-009 4.074e-009 -8.361 -8.390 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.846e-003

HCO3- 2.686e-003 2.500e-003 -2.571 -2.602 -0.031

CaCO3 4.451e-005 4.455e-005 -4.352 -4.351 0.000

CO3-2 4.246e-005 3.185e-005 -4.372 -4.497 -0.125

CaHCO3+ 2.729e-005 2.540e-005 -4.564 -4.595 -0.031

CO2 2.158e-005 2.160e-005 -4.666 -4.665 0.000

MgCO3 1.208e-005 1.209e-005 -4.918 -4.917 0.000

MgHCO3+ 1.185e-005 1.101e-005 -4.926 -4.958 -0.032

NaHCO3 1.303e-008 1.305e-008 -7.885 -7.885 0.000

NaCO3- 7.742e-009 7.191e-009 -8.111 -8.143 -0.032

Ca 1.070e-003

Ca+2 9.868e-004 7.399e-004 -3.006 -3.131 -0.125

CaCO3 4.451e-005 4.455e-005 -4.352 -4.351 0.000

CaHCO3+ 2.729e-005 2.540e-005 -4.564 -4.595 -0.031

CaSO4 1.125e-005 1.126e-005 -4.949 -4.949 0.000

CaOH+ 3.245e-008 3.014e-008 -7.489 -7.521 -0.032

CaHSO4+ 3.105e-013 2.884e-013 -12.508 -12.540 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.316e-005 -4.242 -4.274 -0.032

H(0) 2.227e-028

H2 1.113e-028 1.114e-028 -27.953 -27.953 0.000

K 3.325e-006

K+ 3.324e-006 3.085e-006 -5.478 -5.511 -0.032

KSO4- 1.858e-009 1.725e-009 -8.731 -8.763 -0.032

KOH 2.623e-012 2.626e-012 -11.581 -11.581 0.000

Mg 5.184e-004

Mg+2 4.868e-004 3.662e-004 -3.313 -3.436 -0.124

MgCO3 1.208e-005 1.209e-005 -4.918 -4.917 0.000

MgHCO3+ 1.185e-005 1.101e-005 -4.926 -4.958 -0.032

MgSO4 7.133e-006 7.141e-006 -5.147 -5.146 0.000

MgOH+ 5.672e-007 5.268e-007 -6.246 -6.278 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.279e-006 -5.001 -5.033 -0.032

NaHCO3 1.303e-008 1.305e-008 -7.885 -7.885 0.000

NaCO3- 7.742e-009 7.191e-009 -8.111 -8.143 -0.032

NaSO4- 3.757e-009 3.490e-009 -8.425 -8.457 -0.032

NaOH 1.503e-011 1.505e-011 -10.823 -10.823 0.000

O(0) 6.127e-004

O2 3.063e-004 3.067e-004 -3.514 -3.513 0.000

S(6) 1.154e-004

SO4-2 9.699e-005 7.256e-005 -4.013 -4.139 -0.126

CaSO4 1.125e-005 1.126e-005 -4.949 -4.949 0.000

MgSO4 7.133e-006 7.141e-006 -5.147 -5.146 0.000

NaSO4- 3.757e-009 3.490e-009 -8.425 -8.457 -0.032

KSO4- 1.858e-009 1.725e-009 -8.731 -8.763 -0.032

HSO4- 3.490e-011 3.242e-011 -10.457 -10.489 -0.032

CaHSO4+ 3.105e-013 2.884e-013 -12.508 -12.540 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.74 -7.63 -8.37 CaCO3

Calcite 0.88 -7.63 -8.51 CaCO3

CO2(g) -3.14 -4.67 -1.53 CO2

Dolomite 1.65 -15.56 -17.21 CaMg(CO3)2

Gypsum -2.69 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.78 -27.95 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.58 -3.51 -2.93 O2

Initial solution 112. 30/8/2012 15:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.969e-003 2.969e-003

Ca 1.085e-003 1.085e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.827e-004 5.827e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.390

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 329

Density (g/cm3) = 0.99574

Activity of water = 1.000

Ionic strength = 4.672e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.886e-003

Total CO2 (mol/kg) = 2.886e-003

Temperature (deg C) = 30.400

Electrical balance (eq) = -3.751e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.62

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551590e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8068 0.7111

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.940e-006 3.655e-006 -5.405 -5.437 -0.033

H+ 4.357e-009 4.074e-009 -8.361 -8.390 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.886e-003

HCO3- 2.723e-003 2.533e-003 -2.565 -2.596 -0.031

CaCO3 4.564e-005 4.568e-005 -4.341 -4.340 0.000

CO3-2 4.307e-005 3.228e-005 -4.366 -4.491 -0.125

CaHCO3+ 2.799e-005 2.605e-005 -4.553 -4.584 -0.031

CO2 2.187e-005 2.189e-005 -4.660 -4.660 0.000

MgCO3 1.222e-005 1.223e-005 -4.913 -4.913 0.000

MgHCO3+ 1.199e-005 1.113e-005 -4.921 -4.953 -0.032

NaHCO3 1.320e-008 1.321e-008 -7.879 -7.879 0.000

NaCO3- 7.844e-009 7.284e-009 -8.105 -8.138 -0.032

Ca 1.085e-003

Ca+2 9.998e-004 7.488e-004 -3.000 -3.126 -0.126

CaCO3 4.564e-005 4.568e-005 -4.341 -4.340 0.000

CaHCO3+ 2.799e-005 2.605e-005 -4.553 -4.584 -0.031

CaSO4 1.136e-005 1.137e-005 -4.945 -4.944 0.000

CaOH+ 3.285e-008 3.050e-008 -7.484 -7.516 -0.032

CaHSO4+ 3.136e-013 2.912e-013 -12.504 -12.536 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.314e-005 -4.242 -4.275 -0.033

H(0) 2.227e-028

H2 1.113e-028 1.114e-028 -27.953 -27.953 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.033

KSO4- 1.854e-009 1.721e-009 -8.732 -8.764 -0.032

KOH 2.622e-012 2.625e-012 -11.581 -11.581 0.000

Mg 5.184e-004

Mg+2 4.865e-004 3.656e-004 -3.313 -3.437 -0.124

MgCO3 1.222e-005 1.223e-005 -4.913 -4.913 0.000

MgHCO3+ 1.199e-005 1.113e-005 -4.921 -4.953 -0.032

MgSO4 7.106e-006 7.113e-006 -5.148 -5.148 0.000

MgOH+ 5.664e-007 5.259e-007 -6.247 -6.279 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.320e-008 1.321e-008 -7.879 -7.879 0.000

NaCO3- 7.844e-009 7.284e-009 -8.105 -8.138 -0.032

NaSO4- 3.749e-009 3.481e-009 -8.426 -8.458 -0.032

NaOH 1.503e-011 1.504e-011 -10.823 -10.823 0.000

O(0) 5.827e-004

O2 2.913e-004 2.916e-004 -3.536 -3.535 0.000

S(6) 1.154e-004

SO4-2 9.690e-005 7.241e-005 -4.014 -4.140 -0.127

CaSO4 1.136e-005 1.137e-005 -4.945 -4.944 0.000

MgSO4 7.106e-006 7.113e-006 -5.148 -5.148 0.000

NaSO4- 3.749e-009 3.481e-009 -8.426 -8.458 -0.032

KSO4- 1.854e-009 1.721e-009 -8.732 -8.764 -0.032

HSO4- 3.484e-011 3.235e-011 -10.458 -10.490 -0.032

CaHSO4+ 3.136e-013 2.912e-013 -12.504 -12.536 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.76 -7.62 -8.37 CaCO3

Calcite 0.90 -7.62 -8.51 CaCO3

CO2(g) -3.13 -4.66 -1.53 CO2

Dolomite 1.67 -15.54 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.78 -27.95 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.61 -3.54 -2.93 O2

Initial solution 113. 30/8/2012 16:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.820e-004 5.820e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.380

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 329

Density (g/cm3) = 0.99574

Activity of water = 1.000

Ionic strength = 4.663e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.879e-003

Total CO2 (mol/kg) = 2.879e-003

Temperature (deg C) = 30.400

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551588e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8167 0.7117

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.850e-006 3.572e-006 -5.415 -5.447 -0.033

H+ 4.459e-009 4.169e-009 -8.351 -8.380 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.879e-003

HCO3- 2.718e-003 2.529e-003 -2.566 -2.597 -0.031

CaCO3 4.442e-005 4.447e-005 -4.352 -4.352 0.000

CO3-2 4.201e-005 3.149e-005 -4.377 -4.502 -0.125

CaHCO3+ 2.788e-005 2.594e-005 -4.555 -4.586 -0.031

CO2 2.234e-005 2.236e-005 -4.651 -4.650 0.000

MgHCO3+ 1.198e-005 1.112e-005 -4.922 -4.954 -0.032

MgCO3 1.193e-005 1.194e-005 -4.923 -4.923 0.000

NaHCO3 1.318e-008 1.319e-008 -7.880 -7.880 0.000

NaCO3- 7.653e-009 7.107e-009 -8.116 -8.148 -0.032

Ca 1.081e-003

Ca+2 9.974e-004 7.472e-004 -3.001 -3.127 -0.125

CaCO3 4.442e-005 4.447e-005 -4.352 -4.352 0.000

CaHCO3+ 2.788e-005 2.594e-005 -4.555 -4.586 -0.031

CaSO4 1.133e-005 1.135e-005 -4.946 -4.945 0.000

CaOH+ 3.203e-008 2.974e-008 -7.494 -7.527 -0.032

CaHSO4+ 3.203e-013 2.975e-013 -12.494 -12.527 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.275 -0.032

H(0) 2.331e-028

H2 1.166e-028 1.167e-028 -27.933 -27.933 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.854e-009 1.722e-009 -8.732 -8.764 -0.032

KOH 2.562e-012 2.565e-012 -11.591 -11.591 0.000

Mg 5.184e-004

Mg+2 4.868e-004 3.659e-004 -3.313 -3.437 -0.124

MgHCO3+ 1.198e-005 1.112e-005 -4.922 -4.954 -0.032

MgCO3 1.193e-005 1.194e-005 -4.923 -4.923 0.000

MgSO4 7.114e-006 7.122e-006 -5.148 -5.147 0.000

MgOH+ 5.539e-007 5.144e-007 -6.257 -6.289 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.318e-008 1.319e-008 -7.880 -7.880 0.000

NaCO3- 7.653e-009 7.107e-009 -8.116 -8.148 -0.032

NaSO4- 3.750e-009 3.483e-009 -8.426 -8.458 -0.032

NaOH 1.468e-011 1.470e-011 -10.833 -10.833 0.000

O(0) 5.820e-004

O2 2.910e-004 2.913e-004 -3.536 -3.536 0.000

S(6) 1.154e-004

SO4-2 9.691e-005 7.244e-005 -4.014 -4.140 -0.126

CaSO4 1.133e-005 1.135e-005 -4.946 -4.945 0.000

MgSO4 7.114e-006 7.122e-006 -5.148 -5.147 0.000

NaSO4- 3.750e-009 3.483e-009 -8.426 -8.458 -0.032

KSO4- 1.854e-009 1.722e-009 -8.732 -8.764 -0.032

HSO4- 3.566e-011 3.311e-011 -10.448 -10.480 -0.032

CaHSO4+ 3.203e-013 2.975e-013 -12.494 -12.527 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.74 -7.63 -8.37 CaCO3

Calcite 0.88 -7.63 -8.51 CaCO3

CO2(g) -3.12 -4.65 -1.53 CO2

Dolomite 1.65 -15.57 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.76 -27.93 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.61 -3.54 -2.93 O2

Initial solution 114. 30/8/2012 16:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.326e-006 3.326e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.802e-004 5.802e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.400

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 328

Density (g/cm3) = 0.99574

Activity of water = 1.000

Ionic strength = 4.658e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.873e-003

Total CO2 (mol/kg) = 2.873e-003

Temperature (deg C) = 30.400

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551586e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.7964 0.7105

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 4.031e-006 3.740e-006 -5.395 -5.427 -0.033

H+ 4.258e-009 3.981e-009 -8.371 -8.400 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.873e-003

HCO3- 2.710e-003 2.521e-003 -2.567 -2.598 -0.031

CaCO3 4.630e-005 4.635e-005 -4.334 -4.334 0.000

CO3-2 4.385e-005 3.287e-005 -4.358 -4.483 -0.125

CaHCO3+ 2.775e-005 2.582e-005 -4.557 -4.588 -0.031

CO2 2.127e-005 2.129e-005 -4.672 -4.672 0.000

MgCO3 1.244e-005 1.246e-005 -4.905 -4.905 0.000

MgHCO3+ 1.193e-005 1.108e-005 -4.923 -4.956 -0.032

NaHCO3 1.314e-008 1.315e-008 -7.881 -7.881 0.000

NaCO3- 7.989e-009 7.419e-009 -8.098 -8.130 -0.032

Ca 1.081e-003

Ca+2 9.957e-004 7.460e-004 -3.002 -3.127 -0.125

CaCO3 4.630e-005 4.635e-005 -4.334 -4.334 0.000

CaHCO3+ 2.775e-005 2.582e-005 -4.557 -4.588 -0.031

CaSO4 1.132e-005 1.133e-005 -4.946 -4.946 0.000

CaOH+ 3.348e-008 3.109e-008 -7.475 -7.507 -0.032

CaHSO4+ 3.055e-013 2.837e-013 -12.515 -12.547 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.275 -0.032

H(0) 2.126e-028

H2 1.063e-028 1.064e-028 -27.973 -27.973 0.000

K 3.326e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.855e-009 1.723e-009 -8.732 -8.764 -0.032

KOH 2.683e-012 2.686e-012 -11.571 -11.571 0.000

Mg 5.184e-004

Mg+2 4.863e-004 3.655e-004 -3.313 -3.437 -0.124

MgCO3 1.244e-005 1.246e-005 -4.905 -4.905 0.000

MgHCO3+ 1.193e-005 1.108e-005 -4.923 -4.956 -0.032

MgSO4 7.111e-006 7.118e-006 -5.148 -5.148 0.000

MgOH+ 5.795e-007 5.382e-007 -6.237 -6.269 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.314e-008 1.315e-008 -7.881 -7.881 0.000

NaCO3- 7.989e-009 7.419e-009 -8.098 -8.130 -0.032

NaSO4- 3.752e-009 3.484e-009 -8.426 -8.458 -0.032

NaOH 1.538e-011 1.539e-011 -10.813 -10.813 0.000

O(0) 5.802e-004

O2 2.901e-004 2.904e-004 -3.537 -3.537 0.000

S(6) 1.154e-004

SO4-2 9.693e-005 7.246e-005 -4.014 -4.140 -0.126

CaSO4 1.132e-005 1.133e-005 -4.946 -4.946 0.000

MgSO4 7.111e-006 7.118e-006 -5.148 -5.148 0.000

NaSO4- 3.752e-009 3.484e-009 -8.426 -8.458 -0.032

KSO4- 1.855e-009 1.723e-009 -8.732 -8.764 -0.032

HSO4- 3.406e-011 3.163e-011 -10.468 -10.500 -0.032

CaHSO4+ 3.055e-013 2.837e-013 -12.515 -12.547 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.76 -7.61 -8.37 CaCO3

Calcite 0.90 -7.61 -8.51 CaCO3

CO2(g) -3.14 -4.67 -1.53 CO2

Dolomite 1.68 -15.53 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.80 -27.97 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.61 -3.54 -2.93 O2

Initial solution 115. 30/8/2012 16:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.701e-004 4.701e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.390

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 329

Density (g/cm3) = 0.99574

Activity of water = 1.000

Ionic strength = 4.660e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.876e-003

Total CO2 (mol/kg) = 2.876e-003

Temperature (deg C) = 30.400

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551576e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.7835 0.7097

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.940e-006 3.655e-006 -5.405 -5.437 -0.033

H+ 4.357e-009 4.074e-009 -8.361 -8.390 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.876e-003

HCO3- 2.714e-003 2.525e-003 -2.566 -2.598 -0.031

CaCO3 4.535e-005 4.540e-005 -4.343 -4.343 0.000

CO3-2 4.292e-005 3.217e-005 -4.367 -4.493 -0.125

CaHCO3+ 2.782e-005 2.588e-005 -4.556 -4.587 -0.031

CO2 2.180e-005 2.182e-005 -4.662 -4.661 0.000

MgCO3 1.218e-005 1.220e-005 -4.914 -4.914 0.000

MgHCO3+ 1.195e-005 1.110e-005 -4.923 -4.955 -0.032

NaHCO3 1.316e-008 1.317e-008 -7.881 -7.880 0.000

NaCO3- 7.819e-009 7.261e-009 -8.107 -8.139 -0.032

Ca 1.081e-003

Ca+2 9.966e-004 7.466e-004 -3.001 -3.127 -0.125

CaCO3 4.535e-005 4.540e-005 -4.343 -4.343 0.000

CaHCO3+ 2.782e-005 2.588e-005 -4.556 -4.587 -0.031

CaSO4 1.133e-005 1.134e-005 -4.946 -4.945 0.000

CaOH+ 3.275e-008 3.041e-008 -7.485 -7.517 -0.032

CaHSO4+ 3.128e-013 2.905e-013 -12.505 -12.537 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.275 -0.032

H(0) 2.227e-028

H2 1.113e-028 1.114e-028 -27.953 -27.953 0.000

K 3.325e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.855e-009 1.722e-009 -8.732 -8.764 -0.032

KOH 2.622e-012 2.625e-012 -11.581 -11.581 0.000

Mg 5.184e-004

Mg+2 4.866e-004 3.657e-004 -3.313 -3.437 -0.124

MgCO3 1.218e-005 1.220e-005 -4.914 -4.914 0.000

MgHCO3+ 1.195e-005 1.110e-005 -4.923 -4.955 -0.032

MgSO4 7.113e-006 7.120e-006 -5.148 -5.148 0.000

MgOH+ 5.666e-007 5.261e-007 -6.247 -6.279 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.316e-008 1.317e-008 -7.881 -7.880 0.000

NaCO3- 7.819e-009 7.261e-009 -8.107 -8.139 -0.032

NaSO4- 3.751e-009 3.483e-009 -8.426 -8.458 -0.032

NaOH 1.503e-011 1.504e-011 -10.823 -10.823 0.000

O(0) 4.701e-004

O2 2.351e-004 2.353e-004 -3.629 -3.628 0.000

S(6) 1.154e-004

SO4-2 9.692e-005 7.245e-005 -4.014 -4.140 -0.126

CaSO4 1.133e-005 1.134e-005 -4.946 -4.945 0.000

MgSO4 7.113e-006 7.120e-006 -5.148 -5.148 0.000

NaSO4- 3.751e-009 3.483e-009 -8.426 -8.458 -0.032

KSO4- 1.855e-009 1.722e-009 -8.732 -8.764 -0.032

HSO4- 3.485e-011 3.236e-011 -10.458 -10.490 -0.032

CaHSO4+ 3.128e-013 2.905e-013 -12.505 -12.537 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.75 -7.62 -8.37 CaCO3

Calcite 0.89 -7.62 -8.51 CaCO3

CO2(g) -3.13 -4.66 -1.53 CO2

Dolomite 1.66 -15.55 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.78 -27.95 -3.17 H2

H2O(g) -1.37 -0.00 1.37 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.70 -3.63 -2.93 O2

Initial solution 116. 30/8/2012 16:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.949e-003 2.949e-003

Ca 1.077e-003 1.077e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.933e-004 4.933e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.380

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 327

Density (g/cm3) = 0.99577

Activity of water = 1.000

Ionic strength = 4.652e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.869e-003

Total CO2 (mol/kg) = 2.869e-003

Temperature (deg C) = 30.300

Electrical balance (eq) = -3.183e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.52

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551576e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8067 0.7109

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.822e-006 3.547e-006 -5.418 -5.450 -0.033

H+ 4.458e-009 4.169e-009 -8.351 -8.380 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.869e-003

HCO3- 2.709e-003 2.521e-003 -2.567 -2.598 -0.031

CaCO3 4.398e-005 4.403e-005 -4.357 -4.356 0.000

CO3-2 4.179e-005 3.133e-005 -4.379 -4.504 -0.125

CaHCO3+ 2.768e-005 2.576e-005 -4.558 -4.589 -0.031

CO2 2.229e-005 2.231e-005 -4.652 -4.651 0.000

MgHCO3+ 1.194e-005 1.109e-005 -4.923 -4.955 -0.032

MgCO3 1.186e-005 1.187e-005 -4.926 -4.925 0.000

NaHCO3 1.314e-008 1.315e-008 -7.881 -7.881 0.000

NaCO3- 7.579e-009 7.039e-009 -8.120 -8.153 -0.032

Ca 1.077e-003

Ca+2 9.944e-004 7.451e-004 -3.002 -3.128 -0.125

CaCO3 4.398e-005 4.403e-005 -4.357 -4.356 0.000

CaHCO3+ 2.768e-005 2.576e-005 -4.558 -4.589 -0.031

CaSO4 1.130e-005 1.131e-005 -4.947 -4.946 0.000

CaOH+ 3.194e-008 2.966e-008 -7.496 -7.528 -0.032

CaHSO4+ 3.189e-013 2.962e-013 -12.496 -12.528 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.274 -0.032

H(0) 2.334e-028

H2 1.167e-028 1.168e-028 -27.933 -27.933 0.000

K 3.325e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.853e-009 1.721e-009 -8.732 -8.764 -0.032

KOH 2.563e-012 2.565e-012 -11.591 -11.591 0.000

Mg 5.184e-004

Mg+2 4.869e-004 3.661e-004 -3.313 -3.436 -0.124

MgHCO3+ 1.194e-005 1.109e-005 -4.923 -4.955 -0.032

MgCO3 1.186e-005 1.187e-005 -4.926 -4.925 0.000

MgSO4 7.106e-006 7.114e-006 -5.148 -5.148 0.000

MgOH+ 5.494e-007 5.102e-007 -6.260 -6.292 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.314e-008 1.315e-008 -7.881 -7.881 0.000

NaCO3- 7.579e-009 7.039e-009 -8.120 -8.153 -0.032

NaSO4- 3.751e-009 3.484e-009 -8.426 -8.458 -0.032

NaOH 1.469e-011 1.470e-011 -10.833 -10.833 0.000

O(0) 4.933e-004

O2 2.466e-004 2.469e-004 -3.608 -3.607 0.000

S(6) 1.154e-004

SO4-2 9.695e-005 7.249e-005 -4.013 -4.140 -0.126

CaSO4 1.130e-005 1.131e-005 -4.947 -4.946 0.000

MgSO4 7.106e-006 7.114e-006 -5.148 -5.148 0.000

NaSO4- 3.751e-009 3.484e-009 -8.426 -8.458 -0.032

KSO4- 1.853e-009 1.721e-009 -8.732 -8.764 -0.032

HSO4- 3.560e-011 3.306e-011 -10.449 -10.481 -0.032

CaHSO4+ 3.189e-013 2.962e-013 -12.496 -12.528 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.74 -7.63 -8.37 CaCO3

Calcite 0.88 -7.63 -8.51 CaCO3

CO2(g) -3.12 -4.65 -1.53 CO2

Dolomite 1.64 -15.57 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.76 -27.93 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.68 -3.61 -2.93 O2

Initial solution 117. 30/8/2012 17:09:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.689e-004 4.689e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.380

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 328

Density (g/cm3) = 0.99577

Activity of water = 1.000

Ionic strength = 4.664e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.879e-003

Total CO2 (mol/kg) = 2.879e-003

Temperature (deg C) = 30.300

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551577e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8012 0.7105

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.823e-006 3.547e-006 -5.418 -5.450 -0.033

H+ 4.459e-009 4.169e-009 -8.351 -8.380 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.879e-003

HCO3- 2.719e-003 2.530e-003 -2.566 -2.597 -0.031

CaCO3 4.426e-005 4.431e-005 -4.354 -4.353 0.000

CO3-2 4.194e-005 3.144e-005 -4.377 -4.503 -0.125

CaHCO3+ 2.786e-005 2.592e-005 -4.555 -4.586 -0.031

CO2 2.236e-005 2.239e-005 -4.650 -4.650 0.000

MgHCO3+ 1.197e-005 1.112e-005 -4.922 -4.954 -0.032

MgCO3 1.190e-005 1.191e-005 -4.925 -4.924 0.000

NaHCO3 1.318e-008 1.320e-008 -7.880 -7.880 0.000

NaCO3- 7.604e-009 7.062e-009 -8.119 -8.151 -0.032

Ca 1.081e-003

Ca+2 9.976e-004 7.473e-004 -3.001 -3.126 -0.125

CaCO3 4.426e-005 4.431e-005 -4.354 -4.353 0.000

CaHCO3+ 2.786e-005 2.592e-005 -4.555 -4.586 -0.031

CaSO4 1.133e-005 1.134e-005 -4.946 -4.945 0.000

CaOH+ 3.203e-008 2.975e-008 -7.494 -7.527 -0.032

CaHSO4+ 3.197e-013 2.969e-013 -12.495 -12.527 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.275 -0.032

H(0) 2.334e-028

H2 1.167e-028 1.168e-028 -27.933 -27.933 0.000

K 3.325e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.852e-009 1.719e-009 -8.732 -8.765 -0.032

KOH 2.562e-012 2.565e-012 -11.591 -11.591 0.000

Mg 5.184e-004

Mg+2 4.869e-004 3.659e-004 -3.313 -3.437 -0.124

MgHCO3+ 1.197e-005 1.112e-005 -4.922 -4.954 -0.032

MgCO3 1.190e-005 1.191e-005 -4.925 -4.924 0.000

MgSO4 7.100e-006 7.107e-006 -5.149 -5.148 0.000

MgOH+ 5.492e-007 5.100e-007 -6.260 -6.292 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.318e-008 1.320e-008 -7.880 -7.880 0.000

NaCO3- 7.604e-009 7.062e-009 -8.119 -8.151 -0.032

NaSO4- 3.749e-009 3.482e-009 -8.426 -8.458 -0.032

NaOH 1.469e-011 1.470e-011 -10.833 -10.833 0.000

O(0) 4.689e-004

O2 2.344e-004 2.347e-004 -3.630 -3.630 0.000

S(6) 1.154e-004

SO4-2 9.693e-005 7.245e-005 -4.014 -4.140 -0.126

CaSO4 1.133e-005 1.134e-005 -4.946 -4.945 0.000

MgSO4 7.100e-006 7.107e-006 -5.149 -5.148 0.000

NaSO4- 3.749e-009 3.482e-009 -8.426 -8.458 -0.032

KSO4- 1.852e-009 1.719e-009 -8.732 -8.765 -0.032

HSO4- 3.558e-011 3.305e-011 -10.449 -10.481 -0.032

CaHSO4+ 3.197e-013 2.969e-013 -12.495 -12.527 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.74 -7.63 -8.37 CaCO3

Calcite 0.88 -7.63 -8.51 CaCO3

CO2(g) -3.12 -4.65 -1.53 CO2

Dolomite 1.64 -15.57 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.76 -27.93 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.70 -3.63 -2.93 O2

Initial solution 118. 30/8/2012 17:24:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.826e-004 4.826e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.390

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 328

Density (g/cm3) = 0.99577

Activity of water = 1.000

Ionic strength = 4.661e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.876e-003

Total CO2 (mol/kg) = 2.876e-003

Temperature (deg C) = 30.300

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551577e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.7944 0.7101

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.912e-006 3.629e-006 -5.408 -5.440 -0.033

H+ 4.357e-009 4.074e-009 -8.361 -8.390 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.876e-003

HCO3- 2.715e-003 2.526e-003 -2.566 -2.598 -0.031

CaCO3 4.519e-005 4.524e-005 -4.345 -4.345 0.000

CO3-2 4.285e-005 3.212e-005 -4.368 -4.493 -0.125

CaHCO3+ 2.780e-005 2.586e-005 -4.556 -4.587 -0.031

CO2 2.182e-005 2.184e-005 -4.661 -4.661 0.000

MgCO3 1.215e-005 1.216e-005 -4.915 -4.915 0.000

MgHCO3+ 1.195e-005 1.110e-005 -4.923 -4.955 -0.032

NaHCO3 1.316e-008 1.318e-008 -7.881 -7.880 0.000

NaCO3- 7.769e-009 7.215e-009 -8.110 -8.142 -0.032

Ca 1.081e-003

Ca+2 9.968e-004 7.467e-004 -3.001 -3.127 -0.125

CaCO3 4.519e-005 4.524e-005 -4.345 -4.345 0.000

CaHCO3+ 2.780e-005 2.586e-005 -4.556 -4.587 -0.031

CaSO4 1.132e-005 1.133e-005 -4.946 -4.946 0.000

CaOH+ 3.275e-008 3.042e-008 -7.485 -7.517 -0.032

CaHSO4+ 3.122e-013 2.900e-013 -12.506 -12.538 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.275 -0.032

H(0) 2.229e-028

H2 1.114e-028 1.116e-028 -27.953 -27.953 0.000

K 3.325e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.852e-009 1.720e-009 -8.732 -8.765 -0.032

KOH 2.622e-012 2.625e-012 -11.581 -11.581 0.000

Mg 5.184e-004

Mg+2 4.866e-004 3.658e-004 -3.313 -3.437 -0.124

MgCO3 1.215e-005 1.216e-005 -4.915 -4.915 0.000

MgHCO3+ 1.195e-005 1.110e-005 -4.923 -4.955 -0.032

MgSO4 7.098e-006 7.105e-006 -5.149 -5.148 0.000

MgOH+ 5.617e-007 5.217e-007 -6.250 -6.283 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.276e-006 -5.001 -5.033 -0.032

NaHCO3 1.316e-008 1.318e-008 -7.881 -7.880 0.000

NaCO3- 7.769e-009 7.215e-009 -8.110 -8.142 -0.032

NaSO4- 3.750e-009 3.482e-009 -8.426 -8.458 -0.032

NaOH 1.503e-011 1.504e-011 -10.823 -10.823 0.000

O(0) 4.826e-004

O2 2.413e-004 2.416e-004 -3.617 -3.617 0.000

S(6) 1.154e-004

SO4-2 9.694e-005 7.247e-005 -4.013 -4.140 -0.126

CaSO4 1.132e-005 1.133e-005 -4.946 -4.946 0.000

MgSO4 7.098e-006 7.105e-006 -5.149 -5.148 0.000

NaSO4- 3.750e-009 3.482e-009 -8.426 -8.458 -0.032

KSO4- 1.852e-009 1.720e-009 -8.732 -8.765 -0.032

HSO4- 3.478e-011 3.230e-011 -10.459 -10.491 -0.032

CaHSO4+ 3.122e-013 2.900e-013 -12.506 -12.538 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.75 -7.62 -8.37 CaCO3

Calcite 0.89 -7.62 -8.51 CaCO3

CO2(g) -3.13 -4.66 -1.53 CO2

Dolomite 1.66 -15.55 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.78 -27.95 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.69 -3.62 -2.93 O2

Initial solution 119. 30/8/2012 17:39:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.949e-003 2.949e-003

Ca 1.077e-003 1.077e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 4.682e-004 4.682e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.380

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 327

Density (g/cm3) = 0.99580

Activity of water = 1.000

Ionic strength = 4.653e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.869e-003

Total CO2 (mol/kg) = 2.869e-003

Temperature (deg C) = 30.200

Electrical balance (eq) = -3.183e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.52

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551574e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.8091 0.7108

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.795e-006 3.521e-006 -5.421 -5.453 -0.033

H+ 4.458e-009 4.169e-009 -8.351 -8.380 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.869e-003

HCO3- 2.710e-003 2.522e-003 -2.567 -2.598 -0.031

CaCO3 4.382e-005 4.387e-005 -4.358 -4.358 0.000

CO3-2 4.173e-005 3.129e-005 -4.380 -4.505 -0.125

CaHCO3+ 2.766e-005 2.574e-005 -4.558 -4.589 -0.031

CO2 2.231e-005 2.234e-005 -4.651 -4.651 0.000

MgHCO3+ 1.194e-005 1.109e-005 -4.923 -4.955 -0.032

MgCO3 1.183e-005 1.184e-005 -4.927 -4.927 0.000

NaHCO3 1.314e-008 1.316e-008 -7.881 -7.881 0.000

NaCO3- 7.530e-009 6.994e-009 -8.123 -8.155 -0.032

Ca 1.077e-003

Ca+2 9.946e-004 7.453e-004 -3.002 -3.128 -0.125

CaCO3 4.382e-005 4.387e-005 -4.358 -4.358 0.000

CaHCO3+ 2.766e-005 2.574e-005 -4.558 -4.589 -0.031

CaSO4 1.130e-005 1.131e-005 -4.947 -4.947 0.000

CaOH+ 3.194e-008 2.967e-008 -7.496 -7.528 -0.032

CaHSO4+ 3.183e-013 2.957e-013 -12.497 -12.529 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.274 -0.032

H(0) 2.336e-028

H2 1.168e-028 1.169e-028 -27.933 -27.932 0.000

K 3.325e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.850e-009 1.718e-009 -8.733 -8.765 -0.032

KOH 2.563e-012 2.565e-012 -11.591 -11.591 0.000

Mg 5.184e-004

Mg+2 4.870e-004 3.661e-004 -3.312 -3.436 -0.124

MgHCO3+ 1.194e-005 1.109e-005 -4.923 -4.955 -0.032

MgCO3 1.183e-005 1.184e-005 -4.927 -4.927 0.000

MgSO4 7.092e-006 7.099e-006 -5.149 -5.149 0.000

MgOH+ 5.447e-007 5.059e-007 -6.264 -6.296 -0.032

Na 1.001e-005

Na+ 9.983e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.314e-008 1.316e-008 -7.881 -7.881 0.000

NaCO3- 7.530e-009 6.994e-009 -8.123 -8.155 -0.032

NaSO4- 3.750e-009 3.482e-009 -8.426 -8.458 -0.032

NaOH 1.469e-011 1.470e-011 -10.833 -10.833 0.000

O(0) 4.682e-004

O2 2.341e-004 2.344e-004 -3.631 -3.630 0.000

S(6) 1.154e-004

SO4-2 9.697e-005 7.251e-005 -4.013 -4.140 -0.126

CaSO4 1.130e-005 1.131e-005 -4.947 -4.947 0.000

MgSO4 7.092e-006 7.099e-006 -5.149 -5.149 0.000

NaSO4- 3.750e-009 3.482e-009 -8.426 -8.458 -0.032

KSO4- 1.850e-009 1.718e-009 -8.733 -8.765 -0.032

HSO4- 3.553e-011 3.300e-011 -10.449 -10.482 -0.032

CaHSO4+ 3.183e-013 2.957e-013 -12.497 -12.529 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.74 -7.63 -8.37 CaCO3

Calcite 0.88 -7.63 -8.51 CaCO3

CO2(g) -3.12 -4.65 -1.53 CO2

Dolomite 1.64 -15.57 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.76 -27.93 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.70 -3.63 -2.93 O2

Initial solution 120. 30/8/2012 17:54:20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 2.959e-003 2.959e-003

Ca 1.081e-003 1.081e-003

Cl 5.727e-005 5.727e-005

K 3.325e-006 3.325e-006

Mg 5.184e-004 5.184e-004

Na 1.001e-005 1.001e-005

O(0) 5.008e-004 5.008e-004

S(6) 1.154e-004 1.154e-004

----------------------------Description of solution----------------------------

pH = 8.420

pe = 4.000

Specific Conductance (uS/cm, 30 oC) = 327

Density (g/cm3) = 0.99580

Activity of water = 1.000

Ionic strength = 4.654e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 2.868e-003

Total CO2 (mol/kg) = 2.868e-003

Temperature (deg C) = 30.200

Electrical balance (eq) = -3.483e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.57

Iterations = 8

Total H = 1.110152e+002

Total O = 5.551577e+001

---------------------------------Redox couples---------------------------------

Redox couple pe Eh (volts)

O(-2)/O(0) 11.7764 0.7088

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 4.161e-006 3.861e-006 -5.381 -5.413 -0.033

H+ 4.066e-009 3.802e-009 -8.391 -8.420 -0.029

H2O 5.551e+001 9.999e-001 1.744 -0.000 0.000

C(4) 2.868e-003

HCO3- 2.702e-003 2.514e-003 -2.568 -2.600 -0.031

CaCO3 4.790e-005 4.795e-005 -4.320 -4.319 0.000

CO3-2 4.562e-005 3.420e-005 -4.341 -4.466 -0.125

CaHCO3+ 2.757e-005 2.566e-005 -4.559 -4.591 -0.031

CO2 2.029e-005 2.031e-005 -4.693 -4.692 0.000

MgCO3 1.290e-005 1.292e-005 -4.889 -4.889 0.000

MgHCO3+ 1.188e-005 1.103e-005 -4.925 -4.957 -0.032

NaHCO3 1.310e-008 1.312e-008 -7.883 -7.882 0.000

NaCO3- 8.232e-009 7.646e-009 -8.084 -8.117 -0.032

Ca 1.081e-003

Ca+2 9.943e-004 7.451e-004 -3.002 -3.128 -0.125

CaCO3 4.790e-005 4.795e-005 -4.320 -4.319 0.000

CaHCO3+ 2.757e-005 2.566e-005 -4.559 -4.591 -0.031

CaSO4 1.130e-005 1.131e-005 -4.947 -4.947 0.000

CaOH+ 3.502e-008 3.252e-008 -7.456 -7.488 -0.032

CaHSO4+ 2.903e-013 2.696e-013 -12.537 -12.569 -0.032

Cl 5.727e-005

Cl- 5.727e-005 5.315e-005 -4.242 -4.274 -0.032

H(0) 1.943e-028

H2 9.715e-029 9.725e-029 -28.013 -28.012 0.000

K 3.325e-006

K+ 3.324e-006 3.084e-006 -5.478 -5.511 -0.032

KSO4- 1.850e-009 1.718e-009 -8.733 -8.765 -0.032

KOH 2.810e-012 2.813e-012 -11.551 -11.551 0.000

Mg 5.184e-004

Mg+2 4.859e-004 3.653e-004 -3.313 -3.437 -0.124

MgCO3 1.290e-005 1.292e-005 -4.889 -4.889 0.000

MgHCO3+ 1.188e-005 1.103e-005 -4.925 -4.957 -0.032

MgSO4 7.077e-006 7.084e-006 -5.150 -5.150 0.000

MgOH+ 5.959e-007 5.535e-007 -6.225 -6.257 -0.032

Na 1.001e-005

Na+ 9.982e-006 9.277e-006 -5.001 -5.033 -0.032

NaHCO3 1.310e-008 1.312e-008 -7.883 -7.882 0.000

NaCO3- 8.232e-009 7.646e-009 -8.084 -8.117 -0.032

NaSO4- 3.750e-009 3.483e-009 -8.426 -8.458 -0.032

NaOH 1.610e-011 1.612e-011 -10.793 -10.793 0.000

O(0) 5.008e-004

O2 2.504e-004 2.506e-004 -3.601 -3.601 0.000

S(6) 1.154e-004

SO4-2 9.699e-005 7.252e-005 -4.013 -4.140 -0.126

CaSO4 1.130e-005 1.131e-005 -4.947 -4.947 0.000

MgSO4 7.077e-006 7.084e-006 -5.150 -5.150 0.000

NaSO4- 3.750e-009 3.483e-009 -8.426 -8.458 -0.032

KSO4- 1.850e-009 1.718e-009 -8.733 -8.765 -0.032

HSO4- 3.241e-011 3.010e-011 -10.489 -10.521 -0.032

CaHSO4+ 2.903e-013 2.696e-013 -12.537 -12.569 -0.032

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.88 -7.27 -4.39 CaSO4

Aragonite 0.78 -7.59 -8.37 CaCO3

Calcite 0.92 -7.59 -8.51 CaCO3

CO2(g) -3.17 -4.69 -1.53 CO2

Dolomite 1.71 -15.50 -17.21 CaMg(CO3)2

Gypsum -2.68 -7.27 -4.58 CaSO4:2H2O

H2(g) -24.84 -28.01 -3.17 H2

H2O(g) -1.38 -0.00 1.38 H2O

Halite -10.90 -9.31 1.59 NaCl

O2(g) -0.67 -3.60 -2.93 O2

------------------

End of simulation.

------------------

------------------------------------

Reading input data for simulation 2.

------------------------------------

-----------

End of run.

-----------

**D.3. Geochemical model output of Well 3-5**

Input file: C:\Users\huan\Desktop\Phreeqc calculation Konza\3-5 Well\2006 3-5\2006 3-5.pqi

Output file: C:\Users\huan\Desktop\Phreeqc calculation Konza\3-5 Well\2006 3-5\2006 3-5.pqo

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

------------------

Reading data base.

------------------

SOLUTION\_MASTER\_SPECIES

SOLUTION\_SPECIES

PHASES

EXCHANGE\_MASTER\_SPECIES

EXCHANGE\_SPECIES

SURFACE\_MASTER\_SPECIES

SURFACE\_SPECIES

RATES

END

------------------------------------

Reading input data for simulation 1.

------------------------------------

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

SOLUTION 1 Date:06-4-2 3-5

temp 13

pH 7 Calcite 0.788

pe 12.7

redox pe

units ppm

density 1

Ca 95.1

K 0.587

Mg 18.9

Na 6

Al 0.097

Sr 0.73

B 0.023

Ba 0.088

Li 0.022

Si 4.77

N(5) 0.01

S(6) 36.2

Cl 2.38

Alkalinity 336 as HCO3

water 1 # kg

SOLUTION 2 06-5-7

temp 13

pH 7 Calcite 0.68

pe 12.7

redox pe

units ppm

density 1

Ca 94.8

K 0.65

Mg 18.9

Na 6.24

Al 0.03

Sr 0.75

B 0.025

Ba 0.095

Li 0.023

Si 4.86

N(5) 0.022

S(6) 27.7

Cl 2.32

Alkalinity 365 as HCO3

water 1 # kg

SOLUTION 3 06-8-15

temp 13

pH 7 Calcite 0.247

pe 12.7

redox pe

units ppm

density 1

Ca 97.6

K 0.919

Mg 19.2

Na 6.85

Sr 0.81

B 0.037

Ba 0.109

Li 0.024

Si 5.67

N(5) 0.377

S(6) 55.7

Cl 3.34

Alkalinity 334 as HCO3

water 1 # kg

SOLUTION 4 06-9-24

temp 13

pH 7 Calcite 0.158

pe 12.7

redox pe

units ppm

density 1

Ca 104

K 0.908

Mg 20.8

Na 6.95

Sr 0.87

B 0.035

Ba 0.115

Li 0.025

Si 5.69

N(5) 0.032

S(6) 36.1

Cl 2.72

Alkalinity 395 as HCO3

water 1 # kg

SOLUTION 5 06-10-12

temp 13

pH 7 Calcite 0.158

pe 12.7

redox pe

units ppm

density 1

Ca 108.6

K 0.899

Mg 21.6

Na 7.08

Sr 0.88

B 0.035

Ba 0.116

Li 0.025

Si 5.8

N(5) 0.03

S(6) 36.2

Cl 3.26

Alkalinity 414 as HCO3

water 1 # kg

SOLUTION 6 06-11-18

temp 13

pH 7 Calcite 0.259

pe 12.7

redox pe

units ppm

density 1

Ca 103.2

K 0.687

Mg 21

Na 7.03

Sr 0.86

B 0.027

Ba 0.109

Li 0.025

Si 5.17

N(5) 0.036

S(6) 42.1

Cl 3.8

Alkalinity 404 as HCO3

water 1 # kg

SELECTED\_OUTPUT

file C:\Users\huan\Desktop\2006 3-5 selected.out.sel

reset false

ph true

pe true

temperature true

alkalinity true

ionic\_strength true

percent\_error true

molalities Ca+2 Mg+2

saturation\_indices CO2(g) Calcite Aragonite Dolomite

Quartz Chalcedony

-------------------------------------------

Beginning of initial solution calculations.

-------------------------------------------

Initial solution 1. Date:06-4-2 3-5

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 3.597e-006 3.597e-006

Alkalinity 5.509e-003 5.509e-003

B 2.129e-006 2.129e-006

Ba 6.411e-007 6.411e-007

Ca 2.374e-003 2.374e-003

Cl 6.716e-005 6.716e-005

K 1.502e-005 1.502e-005

Li 3.172e-006 3.172e-006

Mg 7.778e-004 7.778e-004

N(5) 7.143e-007 7.143e-007

Na 2.611e-004 2.611e-004

S(6) 3.770e-004 3.770e-004

Si 7.943e-005 7.943e-005

Sr 8.336e-006 8.336e-006

----------------------------Description of solution----------------------------

pH = 7.960 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 427

Density (g/cm3) = 0.99980

Activity of water = 1.000

Ionic strength = 9.393e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 5.575e-003

Total CO2 (mol/kg) = 5.575e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = 2.804e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 2.29

Iterations = 12

Total H = 1.110181e+002

Total O = 5.552465e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.832e-007 3.466e-007 -6.417 -6.460 -0.044

H+ 1.196e-008 1.097e-008 -7.922 -7.960 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 3.597e-006

Al(OH)4- 3.571e-006 3.236e-006 -5.447 -5.490 -0.043

Al(OH)3 2.120e-008 2.124e-008 -7.674 -7.673 0.001

Al(OH)2+ 4.554e-009 4.127e-009 -8.342 -8.384 -0.043

AlOH+2 2.642e-011 1.782e-011 -10.578 -10.749 -0.171

Al+3 9.579e-014 4.386e-014 -13.019 -13.358 -0.339

AlSO4+ 2.689e-014 2.437e-014 -13.570 -13.613 -0.043

Al(SO4)2- 1.658e-016 1.502e-016 -15.780 -15.823 -0.043

AlHSO4+2 3.224e-023 2.175e-023 -22.492 -22.663 -0.171

B 2.129e-006

H3BO3 2.035e-006 2.039e-006 -5.691 -5.691 0.001

H2BO3- 9.395e-008 8.514e-008 -7.027 -7.070 -0.043

Ba 6.411e-007

Ba+2 5.838e-007 3.972e-007 -6.234 -6.401 -0.167

BaSO4 4.104e-008 4.113e-008 -7.387 -7.386 0.001

BaHCO3+ 1.377e-008 1.248e-008 -7.861 -7.904 -0.043

BaCO3 2.481e-009 2.487e-009 -8.605 -8.604 0.001

BaOH+ 1.353e-012 1.227e-012 -11.869 -11.911 -0.043

C(4) 5.575e-003

HCO3- 5.261e-003 4.783e-003 -2.279 -2.320 -0.041

CO2 1.428e-004 1.431e-004 -3.845 -3.844 0.001

CaHCO3+ 7.975e-005 7.250e-005 -4.098 -4.140 -0.041

CaCO3 3.245e-005 3.252e-005 -4.489 -4.488 0.001

MgHCO3+ 2.960e-005 2.682e-005 -4.529 -4.571 -0.043

CO3-2 2.257e-005 1.542e-005 -4.646 -4.812 -0.165

MgCO3 6.078e-006 6.091e-006 -5.216 -5.215 0.001

NaHCO3 6.335e-007 6.349e-007 -6.198 -6.197 0.001

SrHCO3+ 2.857e-007 2.598e-007 -6.544 -6.585 -0.041

NaCO3- 3.981e-008 3.608e-008 -7.400 -7.443 -0.043

SrCO3 3.690e-008 3.698e-008 -7.433 -7.432 0.001

BaHCO3+ 1.377e-008 1.248e-008 -7.861 -7.904 -0.043

BaCO3 2.481e-009 2.487e-009 -8.605 -8.604 0.001

Ca 2.374e-003

Ca+2 2.207e-003 1.507e-003 -2.656 -2.822 -0.166

CaHCO3+ 7.975e-005 7.250e-005 -4.098 -4.140 -0.041

CaSO4 5.515e-005 5.527e-005 -4.258 -4.258 0.001

CaCO3 3.245e-005 3.252e-005 -4.489 -4.488 0.001

CaOH+ 2.515e-008 2.279e-008 -7.600 -7.642 -0.043

CaHSO4+ 3.436e-012 3.114e-012 -11.464 -11.507 -0.043

Cl 6.716e-005

Cl- 6.716e-005 6.077e-005 -4.173 -4.216 -0.043

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -44.416 -44.416 0.001

K 1.502e-005

K+ 1.500e-005 1.357e-005 -4.824 -4.867 -0.043

KSO4- 1.748e-008 1.584e-008 -7.757 -7.800 -0.043

KOH 4.280e-012 4.290e-012 -11.369 -11.368 0.001

Li 3.172e-006

Li+ 3.169e-006 2.886e-006 -5.499 -5.540 -0.041

LiSO4- 2.872e-009 2.603e-009 -8.542 -8.585 -0.043

LiOH 6.012e-012 6.025e-012 -11.221 -11.220 0.001

Mg 7.778e-004

Mg+2 7.246e-004 4.977e-004 -3.140 -3.303 -0.163

MgHCO3+ 2.960e-005 2.682e-005 -4.529 -4.571 -0.043

MgSO4 1.743e-005 1.747e-005 -4.759 -4.758 0.001

MgCO3 6.078e-006 6.091e-006 -5.216 -5.215 0.001

MgOH+ 5.876e-008 5.326e-008 -7.231 -7.274 -0.043

N(5) 7.143e-007

NO3- 7.143e-007 6.451e-007 -6.146 -6.190 -0.044

Na 2.611e-004

Na+ 2.602e-004 2.361e-004 -3.585 -3.627 -0.042

NaHCO3 6.335e-007 6.349e-007 -6.198 -6.197 0.001

NaSO4- 2.492e-007 2.258e-007 -6.604 -6.646 -0.043

NaCO3- 3.981e-008 3.608e-008 -7.400 -7.443 -0.043

NaOH 1.418e-010 1.421e-010 -9.848 -9.847 0.001

O(0) 5.199e-008

O2 2.599e-008 2.605e-008 -7.585 -7.584 0.001

S(6) 3.770e-004

SO4-2 3.039e-004 2.066e-004 -3.517 -3.685 -0.168

CaSO4 5.515e-005 5.527e-005 -4.258 -4.258 0.001

MgSO4 1.743e-005 1.747e-005 -4.759 -4.758 0.001

NaSO4- 2.492e-007 2.258e-007 -6.604 -6.646 -0.043

SrSO4 1.858e-007 1.862e-007 -6.731 -6.730 0.001

BaSO4 4.104e-008 4.113e-008 -7.387 -7.386 0.001

KSO4- 1.748e-008 1.584e-008 -7.757 -7.800 -0.043

LiSO4- 2.872e-009 2.603e-009 -8.542 -8.585 -0.043

HSO4- 1.897e-010 1.719e-010 -9.722 -9.765 -0.043

CaHSO4+ 3.436e-012 3.114e-012 -11.464 -11.507 -0.043

AlSO4+ 2.689e-014 2.437e-014 -13.570 -13.613 -0.043

Al(SO4)2- 1.658e-016 1.502e-016 -15.780 -15.823 -0.043

AlHSO4+2 3.224e-023 2.175e-023 -22.492 -22.663 -0.171

Si 7.943e-005

H4SiO4 7.868e-005 7.885e-005 -4.104 -4.103 0.001

H3SiO4- 7.442e-007 6.744e-007 -6.128 -6.171 -0.043

H2SiO4-2 2.678e-012 1.806e-012 -11.572 -11.743 -0.171

Sr 8.336e-006

Sr+2 7.827e-006 5.354e-006 -5.106 -5.271 -0.165

SrHCO3+ 2.857e-007 2.598e-007 -6.544 -6.585 -0.041

SrSO4 1.858e-007 1.862e-007 -6.731 -6.730 0.001

SrCO3 3.690e-008 3.698e-008 -7.433 -7.432 0.001

SrOH+ 2.756e-011 2.503e-011 -10.560 -10.602 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -1.09 10.52 11.61 Al(OH)3

Albite -2.63 -21.43 -18.80 NaAlSi3O8

Alunite -4.70 -4.55 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.17 -6.51 -4.33 CaSO4

Anorthite -1.94 -22.01 -20.07 CaAl2Si2O8

Aragonite 0.64 -7.63 -8.27 CaCO3

Barite 0.10 -10.09 -10.18 BaSO4

Ca-Montmorillonite 2.59 -44.23 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.79 -7.63 -8.42 CaCO3

Celestite -2.33 -8.96 -6.62 SrSO4

Chalcedony -0.41 -4.10 -3.70 SiO2

Chlorite(14A) -1.22 71.82 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -4.11 29.64 33.75 Mg3Si2O5(OH)4

CO2(g) -2.53 -3.84 -1.31 CO2

Dolomite 1.05 -15.75 -16.80 CaMg(CO3)2

Gibbsite 1.71 10.52 8.81 Al(OH)3

Gypsum -1.92 -6.51 -4.59 CaSO4:2H2O

H2(g) -41.32 -44.42 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.40 -7.84 1.55 NaCl

Illite 1.66 -40.29 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -1.15 -22.67 -21.52 KAlSi3O8

K-mica 7.82 22.35 14.53 KAl3Si3O10(OH)2

Kaolinite 4.32 12.84 8.52 Al2Si2O5(OH)4

O2(g) -4.79 -7.58 -2.79 O2

Quartz 0.06 -4.10 -4.16 SiO2

Sepiolite -3.17 12.92 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -5.74 12.92 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.29 -4.10 -2.81 SiO2

Strontianite -0.80 -10.08 -9.28 SrCO3

Talc -1.39 21.44 22.82 Mg3Si4O10(OH)2

Witherite -2.60 -11.21 -8.61 BaCO3

Initial solution 2. 06-5-7

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 1.112e-006 1.112e-006

Alkalinity 5.985e-003 5.985e-003

B 2.314e-006 2.314e-006

Ba 6.921e-007 6.921e-007

Ca 2.367e-003 2.367e-003

Cl 6.547e-005 6.547e-005

K 1.663e-005 1.663e-005

Li 3.316e-006 3.316e-006

Mg 7.778e-004 7.778e-004

N(5) 1.571e-006 1.571e-006

Na 2.716e-004 2.716e-004

S(6) 2.885e-004 2.885e-004

Si 8.093e-005 8.093e-005

Sr 8.564e-006 8.564e-006

----------------------------Description of solution----------------------------

pH = 7.812 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 436

Density (g/cm3) = 0.99981

Activity of water = 1.000

Ionic strength = 9.517e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.151e-003

Total CO2 (mol/kg) = 6.151e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -2.693e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.21

Iterations = 11

Total H = 1.110187e+002

Total O = 5.552595e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.730e-007 2.468e-007 -6.564 -6.608 -0.044

H+ 1.681e-008 1.540e-008 -7.774 -7.812 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 1.112e-006

Al(OH)4- 1.100e-006 9.968e-007 -5.958 -6.001 -0.043

Al(OH)3 9.168e-009 9.188e-009 -8.038 -8.037 0.001

Al(OH)2+ 2.767e-009 2.507e-009 -8.558 -8.601 -0.043

AlOH+2 2.258e-011 1.520e-011 -10.646 -10.818 -0.172

Al+3 1.152e-013 5.252e-014 -12.939 -13.280 -0.341

AlSO4+ 2.461e-014 2.229e-014 -13.609 -13.652 -0.043

Al(SO4)2- 1.159e-016 1.049e-016 -15.936 -15.979 -0.043

AlHSO4+2 4.149e-023 2.793e-023 -22.382 -22.554 -0.172

B 2.314e-006

H3BO3 2.240e-006 2.245e-006 -5.650 -5.649 0.001

H2BO3- 7.370e-008 6.676e-008 -7.133 -7.176 -0.043

Ba 6.921e-007

Ba+2 6.392e-007 4.340e-007 -6.194 -6.363 -0.168

BaSO4 3.425e-008 3.432e-008 -7.465 -7.464 0.001

BaHCO3+ 1.648e-008 1.493e-008 -7.783 -7.826 -0.043

BaCO3 2.114e-009 2.118e-009 -8.675 -8.674 0.001

BaOH+ 1.054e-012 9.544e-013 -11.977 -12.020 -0.043

C(4) 6.151e-003

HCO3- 5.763e-003 5.237e-003 -2.239 -2.281 -0.042

CO2 2.195e-004 2.200e-004 -3.659 -3.658 0.001

CaHCO3+ 8.737e-005 7.939e-005 -4.059 -4.100 -0.042

MgHCO3+ 3.247e-005 2.941e-005 -4.488 -4.531 -0.043

CaCO3 2.531e-005 2.536e-005 -4.597 -4.596 0.001

CO3-2 1.764e-005 1.202e-005 -4.754 -4.920 -0.166

MgCO3 4.746e-006 4.756e-006 -5.324 -5.323 0.001

NaHCO3 7.210e-007 7.226e-007 -6.142 -6.141 0.001

SrHCO3+ 3.219e-007 2.925e-007 -6.492 -6.534 -0.042

NaCO3- 3.228e-008 2.924e-008 -7.491 -7.534 -0.043

SrCO3 2.959e-008 2.965e-008 -7.529 -7.528 0.001

BaHCO3+ 1.648e-008 1.493e-008 -7.783 -7.826 -0.043

BaCO3 2.114e-009 2.118e-009 -8.675 -8.674 0.001

Ca 2.367e-003

Ca+2 2.212e-003 1.507e-003 -2.655 -2.822 -0.167

CaHCO3+ 8.737e-005 7.939e-005 -4.059 -4.100 -0.042

CaSO4 4.212e-005 4.222e-005 -4.375 -4.375 0.001

CaCO3 2.531e-005 2.536e-005 -4.597 -4.596 0.001

CaOH+ 1.792e-008 1.623e-008 -7.747 -7.790 -0.043

CaHSO4+ 3.688e-012 3.340e-012 -11.433 -11.476 -0.043

Cl 6.547e-005

Cl- 6.547e-005 5.920e-005 -4.184 -4.228 -0.044

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -44.122 -44.121 0.001

K 1.663e-005

K+ 1.662e-005 1.503e-005 -4.779 -4.823 -0.044

KSO4- 1.479e-008 1.339e-008 -7.830 -7.873 -0.043

KOH 3.374e-012 3.382e-012 -11.472 -11.471 0.001

Li 3.316e-006

Li+ 3.314e-006 3.016e-006 -5.480 -5.521 -0.041

LiSO4- 2.294e-009 2.078e-009 -8.639 -8.682 -0.043

LiOH 4.475e-012 4.485e-012 -11.349 -11.348 0.001

Mg 7.778e-004

Mg+2 7.272e-004 4.985e-004 -3.138 -3.302 -0.164

MgHCO3+ 3.247e-005 2.941e-005 -4.488 -4.531 -0.043

MgSO4 1.333e-005 1.336e-005 -4.875 -4.874 0.001

MgCO3 4.746e-006 4.756e-006 -5.324 -5.323 0.001

MgOH+ 4.193e-008 3.798e-008 -7.377 -7.420 -0.043

N(5) 1.571e-006

NO3- 1.571e-006 1.418e-006 -5.804 -5.848 -0.044

Na 2.716e-004

Na+ 2.706e-004 2.454e-004 -3.568 -3.610 -0.043

NaHCO3 7.210e-007 7.226e-007 -6.142 -6.141 0.001

NaSO4- 1.979e-007 1.793e-007 -6.704 -6.746 -0.043

NaCO3- 3.228e-008 2.924e-008 -7.491 -7.534 -0.043

NaOH 1.050e-010 1.052e-010 -9.979 -9.978 0.001

O(0) 1.337e-008

O2 6.685e-009 6.700e-009 -8.175 -8.174 0.001

S(6) 2.885e-004

SO4-2 2.326e-004 1.578e-004 -3.633 -3.802 -0.169

CaSO4 4.212e-005 4.222e-005 -4.375 -4.375 0.001

MgSO4 1.333e-005 1.336e-005 -4.875 -4.874 0.001

NaSO4- 1.979e-007 1.793e-007 -6.704 -6.746 -0.043

SrSO4 1.459e-007 1.462e-007 -6.836 -6.835 0.001

BaSO4 3.425e-008 3.432e-008 -7.465 -7.464 0.001

KSO4- 1.479e-008 1.339e-008 -7.830 -7.873 -0.043

LiSO4- 2.294e-009 2.078e-009 -8.639 -8.682 -0.043

HSO4- 2.036e-010 1.844e-010 -9.691 -9.734 -0.043

CaHSO4+ 3.688e-012 3.340e-012 -11.433 -11.476 -0.043

AlSO4+ 2.461e-014 2.229e-014 -13.609 -13.652 -0.043

Al(SO4)2- 1.159e-016 1.049e-016 -15.936 -15.979 -0.043

AlHSO4+2 4.149e-023 2.793e-023 -22.382 -22.554 -0.172

Si 8.093e-005

H4SiO4 8.039e-005 8.056e-005 -4.095 -4.094 0.001

H3SiO4- 5.418e-007 4.907e-007 -6.266 -6.309 -0.043

H2SiO4-2 1.390e-012 9.359e-013 -11.857 -12.029 -0.172

Sr 8.564e-006

Sr+2 8.067e-006 5.506e-006 -5.093 -5.259 -0.166

SrHCO3+ 3.219e-007 2.925e-007 -6.492 -6.534 -0.042

SrSO4 1.459e-007 1.462e-007 -6.836 -6.835 0.001

SrCO3 2.959e-008 2.965e-008 -7.529 -7.528 0.001

SrOH+ 2.019e-011 1.833e-011 -10.695 -10.737 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -1.46 10.16 11.61 Al(OH)3

Albite -3.09 -21.89 -18.80 NaAlSi3O8

Alunite -5.54 -5.39 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.29 -6.62 -4.33 CaSO4

Anorthite -2.94 -23.01 -20.07 CaAl2Si2O8

Aragonite 0.53 -7.74 -8.27 CaCO3

Barite 0.02 -10.16 -10.18 BaSO4

Ca-Montmorillonite 1.72 -45.10 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.68 -7.74 -8.42 CaCO3

Celestite -2.44 -9.06 -6.62 SrSO4

Chalcedony -0.40 -4.09 -3.70 SiO2

Chlorite(14A) -3.39 69.64 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -4.97 28.78 33.75 Mg3Si2O5(OH)4

CO2(g) -2.34 -3.66 -1.31 CO2

Dolomite 0.84 -15.96 -16.80 CaMg(CO3)2

Gibbsite 1.35 10.16 8.81 Al(OH)3

Gypsum -2.04 -6.62 -4.59 CaSO4:2H2O

H2(g) -41.02 -44.12 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.39 -7.84 1.55 NaCl

Illite 0.72 -41.23 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -1.59 -23.11 -21.52 KAlSi3O8

K-mica 6.65 21.18 14.53 KAl3Si3O10(OH)2

Kaolinite 3.61 12.13 8.52 Al2Si2O5(OH)4

O2(g) -5.38 -8.17 -2.79 O2

Quartz 0.07 -4.09 -4.16 SiO2

Sepiolite -3.73 12.36 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -6.30 12.36 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.28 -4.09 -2.81 SiO2

Strontianite -0.90 -10.18 -9.28 SrCO3

Talc -2.23 20.59 22.82 Mg3Si4O10(OH)2

Witherite -2.67 -11.28 -8.61 BaCO3

Initial solution 3. 06-8-15

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 5.477e-003 5.477e-003

B 3.425e-006 3.425e-006

Ba 7.941e-007 7.941e-007

Ca 2.436e-003 2.436e-003

Cl 9.426e-005 9.426e-005

K 2.351e-005 2.351e-005

Li 3.461e-006 3.461e-006

Mg 7.901e-004 7.901e-004

N(5) 2.693e-005 2.693e-005

Na 2.981e-004 2.981e-004

S(6) 5.801e-004 5.801e-004

Si 9.442e-005 9.442e-005

Sr 9.249e-006 9.249e-006

----------------------------Description of solution----------------------------

pH = 7.408 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 452

Density (g/cm3) = 0.99982

Activity of water = 1.000

Ionic strength = 9.892e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 5.973e-003

Total CO2 (mol/kg) = 5.973e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = 4.028e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.31

Iterations = 9

Total H = 1.110183e+002

Total O = 5.552641e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.077e-007 9.718e-008 -6.968 -7.012 -0.045

H+ 4.275e-008 3.912e-008 -7.369 -7.408 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 3.425e-006

H3BO3 3.381e-006 3.388e-006 -5.471 -5.470 0.001

H2BO3- 4.387e-008 3.967e-008 -7.358 -7.402 -0.044

Ba 7.941e-007

Ba+2 7.020e-007 4.735e-007 -6.154 -6.325 -0.171

BaSO4 7.456e-008 7.473e-008 -7.127 -7.126 0.001

BaHCO3+ 1.663e-008 1.504e-008 -7.779 -7.823 -0.044

BaCO3 8.381e-010 8.400e-010 -9.077 -9.076 0.001

BaOH+ 4.535e-013 4.100e-013 -12.343 -12.387 -0.044

C(4) 5.973e-003

HCO3- 5.328e-003 4.834e-003 -2.273 -2.316 -0.042

CO2 5.146e-004 5.158e-004 -3.289 -3.288 0.001

CaHCO3+ 8.201e-005 7.440e-005 -4.086 -4.128 -0.042

MgHCO3+ 3.003e-005 2.715e-005 -4.522 -4.566 -0.044

CaCO3 9.337e-006 9.358e-006 -5.030 -5.029 0.001

CO3-2 6.451e-006 4.370e-006 -5.190 -5.360 -0.169

MgCO3 1.725e-006 1.729e-006 -5.763 -5.762 0.001

NaHCO3 7.290e-007 7.306e-007 -6.137 -6.136 0.001

SrHCO3+ 3.157e-007 2.864e-007 -6.501 -6.543 -0.042

BaHCO3+ 1.663e-008 1.504e-008 -7.779 -7.823 -0.044

NaCO3- 1.287e-008 1.164e-008 -7.890 -7.934 -0.044

SrCO3 1.141e-008 1.143e-008 -7.943 -7.942 0.001

BaCO3 8.381e-010 8.400e-010 -9.077 -9.076 0.001

Ca 2.436e-003

Ca+2 2.260e-003 1.530e-003 -2.646 -2.815 -0.169

CaSO4 8.534e-005 8.553e-005 -4.069 -4.068 0.001

CaHCO3+ 8.201e-005 7.440e-005 -4.086 -4.128 -0.042

CaCO3 9.337e-006 9.358e-006 -5.030 -5.029 0.001

CaOH+ 7.176e-009 6.489e-009 -8.144 -8.188 -0.044

CaHSO4+ 1.901e-011 1.719e-011 -10.721 -10.765 -0.044

Cl 9.426e-005

Cl- 9.426e-005 8.508e-005 -4.026 -4.070 -0.044

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.312 -43.311 0.001

K 2.351e-005

K+ 2.347e-005 2.119e-005 -4.629 -4.674 -0.044

KSO4- 4.169e-008 3.769e-008 -7.380 -7.424 -0.044

KOH 1.873e-012 1.878e-012 -11.727 -11.726 0.001

Li 3.461e-006

Li+ 3.456e-006 3.140e-006 -5.461 -5.503 -0.042

LiSO4- 4.774e-009 4.317e-009 -8.321 -8.365 -0.044

LiOH 1.834e-012 1.838e-012 -11.737 -11.736 0.001

Mg 7.901e-004

Mg+2 7.318e-004 4.985e-004 -3.136 -3.302 -0.167

MgHCO3+ 3.003e-005 2.715e-005 -4.522 -4.566 -0.044

MgSO4 2.661e-005 2.667e-005 -4.575 -4.574 0.001

MgCO3 1.725e-006 1.729e-006 -5.763 -5.762 0.001

MgOH+ 1.654e-008 1.496e-008 -7.781 -7.825 -0.044

N(5) 2.693e-005

NO3- 2.693e-005 2.426e-005 -4.570 -4.615 -0.045

Na 2.981e-004

Na+ 2.969e-004 2.688e-004 -3.527 -3.571 -0.043

NaHCO3 7.290e-007 7.306e-007 -6.137 -6.136 0.001

NaSO4- 4.334e-007 3.919e-007 -6.363 -6.407 -0.044

NaCO3- 1.287e-008 1.164e-008 -7.890 -7.934 -0.044

NaOH 4.528e-011 4.539e-011 -10.344 -10.343 0.001

O(0) 3.213e-010

O2 1.607e-010 1.610e-010 -9.794 -9.793 0.001

S(6) 5.801e-004

SO4-2 4.673e-004 3.149e-004 -3.330 -3.502 -0.171

CaSO4 8.534e-005 8.553e-005 -4.069 -4.068 0.001

MgSO4 2.661e-005 2.667e-005 -4.575 -4.574 0.001

NaSO4- 4.334e-007 3.919e-007 -6.363 -6.407 -0.044

SrSO4 3.089e-007 3.096e-007 -6.510 -6.509 0.001

BaSO4 7.456e-008 7.473e-008 -7.127 -7.126 0.001

KSO4- 4.169e-008 3.769e-008 -7.380 -7.424 -0.044

LiSO4- 4.774e-009 4.317e-009 -8.321 -8.365 -0.044

HSO4- 1.033e-009 9.344e-010 -8.986 -9.029 -0.044

CaHSO4+ 1.901e-011 1.719e-011 -10.721 -10.765 -0.044

Si 9.442e-005

H4SiO4 9.417e-005 9.438e-005 -4.026 -4.025 0.001

H3SiO4- 2.503e-007 2.263e-007 -6.602 -6.645 -0.044

H2SiO4-2 2.542e-013 1.700e-013 -12.595 -12.770 -0.175

Sr 9.249e-006

Sr+2 8.613e-006 5.842e-006 -5.065 -5.233 -0.169

SrHCO3+ 3.157e-007 2.864e-007 -6.501 -6.543 -0.042

SrSO4 3.089e-007 3.096e-007 -6.510 -6.509 0.001

SrCO3 1.141e-008 1.143e-008 -7.943 -7.942 0.001

SrOH+ 8.449e-012 7.657e-012 -11.073 -11.116 -0.043

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -1.98 -6.32 -4.33 CaSO4

Aragonite 0.09 -8.17 -8.27 CaCO3

Barite 0.36 -9.83 -10.18 BaSO4

Calcite 0.25 -8.17 -8.42 CaCO3

Celestite -2.11 -8.74 -6.62 SrSO4

Chalcedony -0.33 -4.02 -3.70 SiO2

Chrysotile -7.26 26.49 33.75 Mg3Si2O5(OH)4

CO2(g) -1.97 -3.29 -1.31 CO2

Dolomite -0.04 -16.84 -16.80 CaMg(CO3)2

Gypsum -1.73 -6.32 -4.59 CaSO4:2H2O

H2(g) -40.22 -43.31 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.19 -7.64 1.55 NaCl

O2(g) -7.00 -9.79 -2.79 O2

Quartz 0.14 -4.02 -4.16 SiO2

Sepiolite -5.14 10.95 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -7.71 10.95 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.21 -4.02 -2.81 SiO2

Strontianite -1.31 -10.59 -9.28 SrCO3

Talc -4.39 18.44 22.82 Mg3Si4O10(OH)2

Witherite -3.07 -11.68 -8.61 BaCO3

Initial solution 4. 06-9-24

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 6.477e-003 6.477e-003

B 3.240e-006 3.240e-006

Ba 8.378e-007 8.378e-007

Ca 2.596e-003 2.596e-003

Cl 7.677e-005 7.677e-005

K 2.323e-005 2.323e-005

Li 3.605e-006 3.605e-006

Mg 8.560e-004 8.560e-004

N(5) 2.286e-006 2.286e-006

Na 3.025e-004 3.025e-004

S(6) 3.760e-004 3.760e-004

Si 9.475e-005 9.475e-005

Sr 9.935e-006 9.935e-006

----------------------------Description of solution----------------------------

pH = 7.220 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 480

Density (g/cm3) = 0.99986

Activity of water = 1.000

Ionic strength = 1.051e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.399e-003

Total CO2 (mol/kg) = 7.399e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -5.263e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.38

Iterations = 9

Total H = 1.110193e+002

Total O = 5.552938e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 7.007e-008 6.305e-008 -7.154 -7.200 -0.046

H+ 6.602e-008 6.030e-008 -7.180 -7.220 -0.039

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 3.240e-006

H3BO3 3.212e-006 3.220e-006 -5.493 -5.492 0.001

H2BO3- 2.713e-008 2.446e-008 -7.567 -7.611 -0.045

Ba 8.378e-007

Ba+2 7.649e-007 5.106e-007 -6.116 -6.292 -0.176

BaSO4 5.101e-008 5.113e-008 -7.292 -7.291 0.001

BaHCO3+ 2.123e-008 1.914e-008 -7.673 -7.718 -0.045

BaCO3 6.922e-010 6.939e-010 -9.160 -9.159 0.001

BaOH+ 3.181e-013 2.869e-013 -12.497 -12.542 -0.045

C(4) 7.399e-003

HCO3- 6.306e-003 5.706e-003 -2.200 -2.244 -0.043

CO2 9.361e-004 9.384e-004 -3.029 -3.028 0.001

CaHCO3+ 1.032e-004 9.342e-005 -3.986 -4.030 -0.043

MgHCO3+ 3.838e-005 3.461e-005 -4.416 -4.461 -0.045

CaCO3 7.606e-006 7.624e-006 -5.119 -5.118 0.001

CO3-2 4.991e-006 3.347e-006 -5.302 -5.475 -0.174

MgCO3 1.427e-006 1.430e-006 -5.846 -5.845 0.001

NaHCO3 8.709e-007 8.730e-007 -6.060 -6.059 0.001

SrHCO3+ 4.001e-007 3.621e-007 -6.398 -6.441 -0.043

BaHCO3+ 2.123e-008 1.914e-008 -7.673 -7.718 -0.045

NaCO3- 1.001e-008 9.025e-009 -8.000 -8.045 -0.045

SrCO3 9.355e-009 9.378e-009 -8.029 -8.028 0.001

BaCO3 6.922e-010 6.939e-010 -9.160 -9.159 0.001

Ca 2.596e-003

Ca+2 2.428e-003 1.627e-003 -2.615 -2.789 -0.174

CaHCO3+ 1.032e-004 9.342e-005 -3.986 -4.030 -0.043

CaSO4 5.758e-005 5.772e-005 -4.240 -4.239 0.001

CaCO3 7.606e-006 7.624e-006 -5.119 -5.118 0.001

CaOH+ 4.965e-009 4.478e-009 -8.304 -8.349 -0.045

CaHSO4+ 1.982e-011 1.788e-011 -10.703 -10.748 -0.045

Cl 7.677e-005

Cl- 7.677e-005 6.910e-005 -4.115 -4.161 -0.046

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -42.936 -42.935 0.001

K 2.323e-005

K+ 2.321e-005 2.089e-005 -4.634 -4.680 -0.046

KSO4- 2.615e-008 2.358e-008 -7.583 -7.627 -0.045

KOH 1.198e-012 1.201e-012 -11.921 -11.920 0.001

Li 3.605e-006

Li+ 3.602e-006 3.265e-006 -5.443 -5.486 -0.043

LiSO4- 3.158e-009 2.848e-009 -8.501 -8.546 -0.045

LiOH 1.237e-012 1.240e-012 -11.908 -11.907 0.001

Mg 8.560e-004

Mg+2 7.980e-004 5.383e-004 -3.098 -3.269 -0.171

MgHCO3+ 3.838e-005 3.461e-005 -4.416 -4.461 -0.045

MgSO4 1.823e-005 1.827e-005 -4.739 -4.738 0.001

MgCO3 1.427e-006 1.430e-006 -5.846 -5.845 0.001

MgOH+ 1.162e-008 1.048e-008 -7.935 -7.980 -0.045

N(5) 2.286e-006

NO3- 2.286e-006 2.054e-006 -5.641 -5.687 -0.047

Na 3.025e-004

Na+ 3.013e-004 2.720e-004 -3.521 -3.565 -0.044

NaHCO3 8.709e-007 8.730e-007 -6.060 -6.059 0.001

NaSO4- 2.791e-007 2.517e-007 -6.554 -6.599 -0.045

NaCO3- 1.001e-008 9.025e-009 -8.000 -8.045 -0.045

NaOH 2.973e-011 2.980e-011 -10.527 -10.526 0.001

O(0) 5.694e-011

O2 2.847e-011 2.854e-011 -10.546 -10.545 0.001

S(6) 3.760e-004

SO4-2 2.996e-004 1.998e-004 -3.523 -3.699 -0.176

CaSO4 5.758e-005 5.772e-005 -4.240 -4.239 0.001

MgSO4 1.823e-005 1.827e-005 -4.739 -4.738 0.001

NaSO4- 2.791e-007 2.517e-007 -6.554 -6.599 -0.045

SrSO4 2.098e-007 2.104e-007 -6.678 -6.677 0.001

BaSO4 5.101e-008 5.113e-008 -7.292 -7.291 0.001

KSO4- 2.615e-008 2.358e-008 -7.583 -7.627 -0.045

LiSO4- 3.158e-009 2.848e-009 -8.501 -8.546 -0.045

HSO4- 1.013e-009 9.138e-010 -8.994 -9.039 -0.045

CaHSO4+ 1.982e-011 1.788e-011 -10.703 -10.748 -0.045

Si 9.475e-005

H4SiO4 9.459e-005 9.482e-005 -4.024 -4.023 0.001

H3SiO4- 1.636e-007 1.475e-007 -6.786 -6.831 -0.045

H2SiO4-2 1.087e-013 7.189e-014 -12.964 -13.143 -0.180

Sr 9.935e-006

Sr+2 9.316e-006 6.255e-006 -5.031 -5.204 -0.173

SrHCO3+ 4.001e-007 3.621e-007 -6.398 -6.441 -0.043

SrSO4 2.098e-007 2.104e-007 -6.678 -6.677 0.001

SrCO3 9.355e-009 9.378e-009 -8.029 -8.028 0.001

SrOH+ 5.885e-012 5.320e-012 -11.230 -11.274 -0.044

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.15 -6.49 -4.33 CaSO4

Aragonite 0.01 -8.26 -8.27 CaCO3

Barite 0.19 -9.99 -10.18 BaSO4

Calcite 0.16 -8.26 -8.42 CaCO3

Celestite -2.28 -8.90 -6.62 SrSO4

Chalcedony -0.33 -4.02 -3.70 SiO2

Chrysotile -8.28 25.47 33.75 Mg3Si2O5(OH)4

CO2(g) -1.71 -3.03 -1.31 CO2

Dolomite -0.21 -17.01 -16.80 CaMg(CO3)2

Gypsum -1.90 -6.49 -4.59 CaSO4:2H2O

H2(g) -39.84 -42.94 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.28 -7.73 1.55 NaCl

O2(g) -7.75 -10.54 -2.79 O2

Quartz 0.14 -4.02 -4.16 SiO2

Sepiolite -5.82 10.27 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.39 10.27 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.21 -4.02 -2.81 SiO2

Strontianite -1.40 -10.68 -9.28 SrCO3

Talc -5.40 17.42 22.82 Mg3Si4O10(OH)2

Witherite -3.16 -11.77 -8.61 BaCO3

Initial solution 5. 06-10-12

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 6.789e-003 6.789e-003

B 3.240e-006 3.240e-006

Ba 8.451e-007 8.451e-007

Ca 2.711e-003 2.711e-003

Cl 9.201e-005 9.201e-005

K 2.300e-005 2.300e-005

Li 3.605e-006 3.605e-006

Mg 8.890e-004 8.890e-004

N(5) 2.143e-006 2.143e-006

Na 3.081e-004 3.081e-004

S(6) 3.771e-004 3.771e-004

Si 9.659e-005 9.659e-005

Sr 1.005e-005 1.005e-005

----------------------------Description of solution----------------------------

pH = 7.185 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 499

Density (g/cm3) = 0.99988

Activity of water = 1.000

Ionic strength = 1.094e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.835e-003

Total CO2 (mol/kg) = 7.835e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -8.017e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.55

Iterations = 9

Total H = 1.110196e+002

Total O = 5.553057e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

H+ 7.162e-008 6.532e-008 -7.145 -7.185 -0.040

OH- 6.480e-008 5.820e-008 -7.188 -7.235 -0.047

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 3.240e-006

H3BO3 3.215e-006 3.223e-006 -5.493 -5.492 0.001

H2BO3- 2.510e-008 2.260e-008 -7.600 -7.646 -0.046

Ba 8.451e-007

Ba+2 7.716e-007 5.114e-007 -6.113 -6.291 -0.179

BaSO4 5.059e-008 5.072e-008 -7.296 -7.295 0.001

BaHCO3+ 2.228e-008 2.005e-008 -7.652 -7.698 -0.046

BaCO3 6.692e-010 6.709e-010 -9.174 -9.173 0.001

BaOH+ 2.947e-013 2.652e-013 -12.531 -12.576 -0.046

C(4) 7.835e-003

HCO3- 6.606e-003 5.968e-003 -2.180 -2.224 -0.044

CO2 1.061e-003 1.063e-003 -2.974 -2.973 0.001

CaHCO3+ 1.120e-004 1.012e-004 -3.951 -3.995 -0.044

MgHCO3+ 4.143e-005 3.729e-005 -4.383 -4.428 -0.046

CaCO3 7.605e-006 7.624e-006 -5.119 -5.118 0.001

CO3-2 4.851e-006 3.231e-006 -5.314 -5.491 -0.177

MgCO3 1.419e-006 1.422e-006 -5.848 -5.847 0.001

NaHCO3 9.259e-007 9.283e-007 -6.033 -6.032 0.001

SrHCO3+ 4.206e-007 3.800e-007 -6.376 -6.420 -0.044

BaHCO3+ 2.228e-008 2.005e-008 -7.652 -7.698 -0.046

NaCO3- 9.841e-009 8.858e-009 -8.007 -8.053 -0.046

SrCO3 9.060e-009 9.083e-009 -8.043 -8.042 0.001

BaCO3 6.692e-010 6.709e-010 -9.174 -9.173 0.001

Ca 2.711e-003

Ca+2 2.532e-003 1.686e-003 -2.596 -2.773 -0.177

CaHCO3+ 1.120e-004 1.012e-004 -3.951 -3.995 -0.044

CaSO4 5.907e-005 5.922e-005 -4.229 -4.228 0.001

CaCO3 7.605e-006 7.624e-006 -5.119 -5.118 0.001

CaOH+ 4.756e-009 4.282e-009 -8.323 -8.368 -0.046

CaHSO4+ 2.207e-011 1.987e-011 -10.656 -10.702 -0.046

Cl 9.201e-005

Cl- 9.201e-005 8.266e-005 -4.036 -4.083 -0.047

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -42.867 -42.866 0.001

K 2.300e-005

K+ 2.298e-005 2.064e-005 -4.639 -4.685 -0.047

KSO4- 2.564e-008 2.308e-008 -7.591 -7.637 -0.046

KOH 1.093e-012 1.096e-012 -11.961 -11.960 0.001

Li 3.605e-006

Li+ 3.602e-006 3.259e-006 -5.443 -5.487 -0.043

LiSO4- 3.128e-009 2.815e-009 -8.505 -8.550 -0.046

LiOH 1.140e-012 1.143e-012 -11.943 -11.942 0.001

Mg 8.890e-004

Mg+2 8.275e-004 5.546e-004 -3.082 -3.256 -0.174

MgHCO3+ 4.143e-005 3.729e-005 -4.383 -4.428 -0.046

MgSO4 1.860e-005 1.864e-005 -4.731 -4.730 0.001

MgCO3 1.419e-006 1.422e-006 -5.848 -5.847 0.001

MgOH+ 1.107e-008 9.964e-009 -7.956 -8.002 -0.046

N(5) 2.143e-006

NO3- 2.143e-006 1.921e-006 -5.669 -5.716 -0.047

Na 3.081e-004

Na+ 3.069e-004 2.766e-004 -3.513 -3.558 -0.045

NaHCO3 9.259e-007 9.283e-007 -6.033 -6.032 0.001

NaSO4- 2.815e-007 2.534e-007 -6.550 -6.596 -0.046

NaCO3- 9.841e-009 8.858e-009 -8.007 -8.053 -0.046

NaOH 2.790e-011 2.797e-011 -10.554 -10.553 0.001

O(0) 4.133e-011

O2 2.066e-011 2.072e-011 -10.685 -10.684 0.001

S(6) 3.771e-004

SO4-2 2.988e-004 1.979e-004 -3.525 -3.704 -0.179

CaSO4 5.907e-005 5.922e-005 -4.229 -4.228 0.001

MgSO4 1.860e-005 1.864e-005 -4.731 -4.730 0.001

NaSO4- 2.815e-007 2.534e-007 -6.550 -6.596 -0.046

SrSO4 2.085e-007 2.090e-007 -6.681 -6.680 0.001

BaSO4 5.059e-008 5.072e-008 -7.296 -7.295 0.001

KSO4- 2.564e-008 2.308e-008 -7.591 -7.637 -0.046

LiSO4- 3.128e-009 2.815e-009 -8.505 -8.550 -0.046

HSO4- 1.089e-009 9.804e-010 -8.963 -9.009 -0.046

CaHSO4+ 2.207e-011 1.987e-011 -10.656 -10.702 -0.046

Si 9.659e-005

H4SiO4 9.643e-005 9.668e-005 -4.016 -4.015 0.001

H3SiO4- 1.543e-007 1.389e-007 -6.812 -6.857 -0.046

H2SiO4-2 9.512e-014 6.245e-014 -13.022 -13.204 -0.183

Sr 1.005e-005

Sr+2 9.411e-006 6.277e-006 -5.026 -5.202 -0.176

SrHCO3+ 4.206e-007 3.800e-007 -6.376 -6.420 -0.044

SrSO4 2.085e-007 2.090e-007 -6.681 -6.680 0.001

SrCO3 9.060e-009 9.083e-009 -8.043 -8.042 0.001

SrOH+ 5.460e-012 4.927e-012 -11.263 -11.307 -0.045

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.14 -6.48 -4.33 CaSO4

Aragonite 0.01 -8.26 -8.27 CaCO3

Barite 0.19 -9.99 -10.18 BaSO4

Calcite 0.16 -8.26 -8.42 CaCO3

Celestite -2.28 -8.91 -6.62 SrSO4

Chalcedony -0.32 -4.01 -3.70 SiO2

Chrysotile -8.44 25.31 33.75 Mg3Si2O5(OH)4

CO2(g) -1.66 -2.97 -1.31 CO2

Dolomite -0.21 -17.01 -16.80 CaMg(CO3)2

Gypsum -1.89 -6.48 -4.59 CaSO4:2H2O

H2(g) -39.77 -42.87 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.19 -7.64 1.55 NaCl

O2(g) -7.89 -10.68 -2.79 O2

Quartz 0.15 -4.01 -4.16 SiO2

Sepiolite -5.91 10.18 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.48 10.18 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.20 -4.01 -2.81 SiO2

Strontianite -1.41 -10.69 -9.28 SrCO3

Talc -5.54 17.28 22.82 Mg3Si4O10(OH)2

Witherite -3.17 -11.78 -8.61 BaCO3

Initial solution 6. 06-11-18

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 6.625e-003 6.625e-003

B 2.499e-006 2.499e-006

Ba 7.941e-007 7.941e-007

Ca 2.576e-003 2.576e-003

Cl 1.072e-004 1.072e-004

K 1.758e-005 1.758e-005

Li 3.605e-006 3.605e-006

Mg 8.643e-004 8.643e-004

N(5) 2.572e-006 2.572e-006

Na 3.060e-004 3.060e-004

S(6) 4.385e-004 4.385e-004

Si 8.610e-005 8.610e-005

Sr 9.821e-006 9.821e-006

----------------------------Description of solution----------------------------

pH = 7.318 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 489

Density (g/cm3) = 0.99987

Activity of water = 1.000

Ionic strength = 1.064e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.369e-003

Total CO2 (mol/kg) = 7.369e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -3.819e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.70

Iterations = 9

Total H = 1.110194e+002

Total O = 5.552968e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.793e-008 7.908e-008 -7.056 -7.102 -0.046

H+ 5.266e-008 4.808e-008 -7.279 -7.318 -0.040

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 2.499e-006

H3BO3 2.473e-006 2.479e-006 -5.607 -5.606 0.001

H2BO3- 2.620e-008 2.362e-008 -7.582 -7.627 -0.045

Ba 7.941e-007

Ba+2 7.173e-007 4.778e-007 -6.144 -6.321 -0.176

BaSO4 5.569e-008 5.582e-008 -7.254 -7.253 0.001

BaHCO3+ 2.030e-008 1.830e-008 -7.693 -7.738 -0.045

BaCO3 8.297e-010 8.317e-010 -9.081 -9.080 0.001

BaOH+ 3.735e-013 3.367e-013 -12.428 -12.473 -0.045

C(4) 7.369e-003

HCO3- 6.444e-003 5.828e-003 -2.191 -2.234 -0.044

CO2 7.624e-004 7.642e-004 -3.118 -3.117 0.001

CaHCO3+ 1.039e-004 9.399e-005 -3.983 -4.027 -0.044

MgHCO3+ 3.933e-005 3.545e-005 -4.405 -4.450 -0.045

CaCO3 9.597e-006 9.620e-006 -5.018 -5.017 0.001

CO3-2 6.408e-006 4.288e-006 -5.193 -5.368 -0.174

MgCO3 1.832e-006 1.837e-006 -5.737 -5.736 0.001

NaHCO3 8.990e-007 9.012e-007 -6.046 -6.045 0.001

SrHCO3+ 4.015e-007 3.632e-007 -6.396 -6.440 -0.044

BaHCO3+ 2.030e-008 1.830e-008 -7.693 -7.738 -0.045

NaCO3- 1.296e-008 1.169e-008 -7.887 -7.932 -0.045

SrCO3 1.177e-008 1.180e-008 -7.929 -7.928 0.001

BaCO3 8.297e-010 8.317e-010 -9.081 -9.080 0.001

Ca 2.576e-003

Ca+2 2.397e-003 1.603e-003 -2.620 -2.795 -0.175

CaHCO3+ 1.039e-004 9.399e-005 -3.983 -4.027 -0.044

CaSO4 6.618e-005 6.634e-005 -4.179 -4.178 0.001

CaCO3 9.597e-006 9.620e-006 -5.018 -5.017 0.001

CaOH+ 6.138e-009 5.532e-009 -8.212 -8.257 -0.045

CaHSO4+ 1.818e-011 1.638e-011 -10.741 -10.786 -0.045

Cl 1.072e-004

Cl- 1.072e-004 9.648e-005 -3.970 -4.016 -0.046

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.133 -43.132 0.001

K 1.758e-005

K+ 1.756e-005 1.579e-005 -4.756 -4.802 -0.046

KSO4- 2.308e-008 2.080e-008 -7.637 -7.682 -0.045

KOH 1.136e-012 1.139e-012 -11.945 -11.944 0.001

Li 3.605e-006

Li+ 3.601e-006 3.263e-006 -5.444 -5.486 -0.043

LiSO4- 3.684e-009 3.320e-009 -8.434 -8.479 -0.045

LiOH 1.551e-012 1.554e-012 -11.810 -11.808 0.001

Mg 8.643e-004

Mg+2 8.018e-004 5.398e-004 -3.096 -3.268 -0.172

MgHCO3+ 3.933e-005 3.545e-005 -4.405 -4.450 -0.045

MgSO4 2.133e-005 2.138e-005 -4.671 -4.670 0.001

MgCO3 1.832e-006 1.837e-006 -5.737 -5.736 0.001

MgOH+ 1.462e-008 1.318e-008 -7.835 -7.880 -0.045

N(5) 2.572e-006

NO3- 2.572e-006 2.309e-006 -5.590 -5.637 -0.047

Na 3.060e-004

Na+ 3.047e-004 2.750e-004 -3.516 -3.561 -0.045

NaHCO3 8.990e-007 9.012e-007 -6.046 -6.045 0.001

NaSO4- 3.293e-007 2.968e-007 -6.482 -6.528 -0.045

NaCO3- 1.296e-008 1.169e-008 -7.887 -7.932 -0.045

NaOH 3.769e-011 3.778e-011 -10.424 -10.423 0.001

O(0) 1.409e-010

O2 7.044e-011 7.061e-011 -10.152 -10.151 0.001

S(6) 4.385e-004

SO4-2 3.504e-004 2.331e-004 -3.455 -3.632 -0.177

CaSO4 6.618e-005 6.634e-005 -4.179 -4.178 0.001

MgSO4 2.133e-005 2.138e-005 -4.671 -4.670 0.001

NaSO4- 3.293e-007 2.968e-007 -6.482 -6.528 -0.045

SrSO4 2.404e-007 2.410e-007 -6.619 -6.618 0.001

BaSO4 5.569e-008 5.582e-008 -7.254 -7.253 0.001

KSO4- 2.308e-008 2.080e-008 -7.637 -7.682 -0.045

LiSO4- 3.684e-009 3.320e-009 -8.434 -8.479 -0.045

HSO4- 9.432e-010 8.501e-010 -9.025 -9.071 -0.045

CaHSO4+ 1.818e-011 1.638e-011 -10.741 -10.786 -0.045

Si 8.610e-005

H4SiO4 8.591e-005 8.612e-005 -4.066 -4.065 0.001

H3SiO4- 1.865e-007 1.681e-007 -6.729 -6.775 -0.045

H2SiO4-2 1.556e-013 1.027e-013 -12.808 -12.988 -0.181

Sr 9.821e-006

Sr+2 9.167e-006 6.143e-006 -5.038 -5.212 -0.174

SrHCO3+ 4.015e-007 3.632e-007 -6.396 -6.440 -0.044

SrSO4 2.404e-007 2.410e-007 -6.619 -6.618 0.001

SrCO3 1.177e-008 1.180e-008 -7.929 -7.928 0.001

SrOH+ 7.252e-012 6.551e-012 -11.140 -11.184 -0.044

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.09 -6.43 -4.33 CaSO4

Aragonite 0.11 -8.16 -8.27 CaCO3

Barite 0.23 -9.95 -10.18 BaSO4

Calcite 0.26 -8.16 -8.42 CaCO3

Celestite -2.22 -8.84 -6.62 SrSO4

Chalcedony -0.37 -4.06 -3.70 SiO2

Chrysotile -7.77 25.98 33.75 Mg3Si2O5(OH)4

CO2(g) -1.80 -3.12 -1.31 CO2

Dolomite 0.00 -16.80 -16.80 CaMg(CO3)2

Gypsum -1.84 -6.43 -4.59 CaSO4:2H2O

H2(g) -40.04 -43.13 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.13 -7.58 1.55 NaCl

O2(g) -7.36 -10.15 -2.79 O2

Quartz 0.10 -4.06 -4.16 SiO2

Sepiolite -5.55 10.54 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.12 10.54 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.25 -4.06 -2.81 SiO2

Strontianite -1.30 -10.58 -9.28 SrCO3

Talc -4.98 17.85 22.82 Mg3Si4O10(OH)2

Witherite -3.08 -11.69 -8.61 BaCO3

------------------

End of simulation.

------------------

------------------------------------

Reading input data for simulation 2.

------------------------------------

-----------

End of run.

Input file: C:\Users\huan\Desktop\Phreeqc calculation Konza\3-5 Well\2007 3-5\2007 3-5.pqi

Output file: C:\Users\huan\Desktop\Phreeqc calculation Konza\3-5 Well\2007 3-5\2007 3-5.pqo

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

------------------

Reading data base.

------------------

SOLUTION\_MASTER\_SPECIES

SOLUTION\_SPECIES

PHASES

EXCHANGE\_MASTER\_SPECIES

EXCHANGE\_SPECIES

SURFACE\_MASTER\_SPECIES

SURFACE\_SPECIES

RATES

END

------------------------------------

Reading input data for simulation 1.

------------------------------------

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

SOLUTION 1 07-1-4

temp 13

pH 7 Calcite 0.622

pe 12.7

redox pe

units ppm

density 1

Ca 107.3

K 0.638

Mg 21.7

Na 7.12

Sr 0.88

B 0.022

Ba 0.107

Li 0.023

Si 4.85

N(5) 0.027

S(6) 47.6

Cl 2.7

Alkalinity 459 as HCO3

water 1 # kg

SOLUTION 2 07-2-18

temp 13

pH 7 calcite 0.806

pe 12.7

redox pe

units ppm

density 1

Ca 94.2

K 0.688

Mg 19.8

Na 6.25

Sr 0.78

B 0.017

Ba 0.089

Li 0.021

Si 3.86

S(6) 45.4

Cl 3.04

Alkalinity 348 as HCO3

water 1 # kg

SOLUTION 3 07-3-18

temp 13

pH 7 Calcite 0.812

pe 12.7

redox pe

units ppm

density 1

Ca 94.5

K 0.614

Mg 20.4

Na 6.5

Sr 0.79

B 0.018

Ba 0.093

Li 0.02

Si 4.43

N(5) 0.021

S(6) 38.1

Cl 2.83

Alkalinity 364 as HCO3

water 1 # kg

SOLUTION 4 07-4-22

temp 13

pH 7 Calcite 0.734

pe 12.7

redox pe

units ppm

density 1

Ca 92.2

K 0.771

Mg 19.3

Na 4.46

Al 0.431

Sr 0.84

B 0.028

Ba 0.103

Li 0.026

Si 6.06

N(5) 0.016

S(6) 19.6

Cl 2.73

Alkalinity 359 as HCO3

water 1 # kg

SOLUTION 5 07-6-4

temp 13

pH 7 Calcite 0.56

pe 12.7

redox pe

units ppm

density 1

Ca 86.4

K 0.762

Mg 17.9

Na 4.32

Al 0.001

Sr 0.8

B 0.032

Ba 0.102

Li 0.026

Si 5.68

N(5) 0.02

S(6) 14.2

Cl 2.13

Alkalinity 355 as HCO3

water 1 # kg

SOLUTION 6 07-7-24

temp 13

pH 7 Calcite 0.331

pe 12.7

redox pe

units ppm

density 1

Ca 99.7

K 0.947

Mg 19.6

Na 4.68

Al 0.009

Sr 0.92

B 0.042

Ba 0.123

Li 0.029

Si 6.45

S(6) 24.2

Cl 2.51

Alkalinity 411 as HCO3

water 1 # kg

SOLUTION 7 07-8-26

temp 13

pH 7 Calcite 0.213

pe 12.7

redox pe

units ppm

density 1

Ca 81.9

K 1.166

Mg 26.2

Na 5.88

Al 0

Sr 1.52

B 0.036

Ba 0.054

Li 0.032

Si 5.69

N(5) 0.027

S(6) 38.9

Cl 3.12

Alkalinity 359 as HCO3

water 1 # kg

SOLUTION 8 07-9-22

temp 13

pH 7 Calcite 0.16

pe 12.7

redox pe

units ppm

density 1

Ca 95.7

K 1.006

Mg 19.7

Na 4.61

Al 0.093

Sr 0.85

B 0.056

Ba 0.119

Li 0.03

Si 5.94

N(5) 0.045

S(6) 35.7

Cl 2.41

Alkalinity 374 as HCO3

water 1 # kg

SOLUTION 9 07-10-28

temp 13

pH 7 Calcite 0.183

pe 12.7

redox pe

units ppm

density 1

Ca 103.1

K 0.94

Mg 19.9

Na 4.84

Al 0.004

Sr 0.95

B 0.037

Ba 0.125

Li 0.029

Si 6.26

N(5) 0.031

S(6) 44.6

Cl 2.68

Alkalinity 374 as HCO3

water 1 # kg

SOLUTION 10 07-11-18

temp 13

pH 7 Calcite 0.259

pe 12.7

redox pe

units ppm

density 1

Ca 108.3

K 0.924

Mg 21.8

Na 5

Al 0.019

Sr 0.97

B 0.037

Ba 0.122

Li 0.029

Si 6.03

S(6) 45.2

Cl 2.4

Alkalinity 390 as HCO3

water 1 # kg

SELECTED\_OUTPUT

file C:\Users\huan\Desktop\2007 3-5 selected.out.sel

reset false

ph true

pe true

temperature true

alkalinity true

ionic\_strength true

percent\_error true

molalities Ca+2 Mg+2

saturation\_indices CO2(g) Calcite Aragonite Dolomite

Quartz Chalcedony

-------------------------------------------

Beginning of initial solution calculations.

-------------------------------------------

Initial solution 1. 07-1-4

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 7.527e-003 7.527e-003

B 2.036e-006 2.036e-006

Ba 7.796e-007 7.796e-007

Ca 2.679e-003 2.679e-003

Cl 7.621e-005 7.621e-005

K 1.633e-005 1.633e-005

Li 3.317e-006 3.317e-006

Mg 8.931e-004 8.931e-004

N(5) 1.929e-006 1.929e-006

Na 3.099e-004 3.099e-004

S(6) 4.958e-004 4.958e-004

Si 8.077e-005 8.077e-005

Sr 1.005e-005 1.005e-005

----------------------------Description of solution----------------------------

pH = 7.622 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 523

Density (g/cm3) = 0.99991

Activity of water = 1.000

Ionic strength = 1.133e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.912e-003

Total CO2 (mol/kg) = 7.912e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -1.102e-003

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -7.22

Iterations = 9

Total H = 1.110202e+002

Total O = 5.553184e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.777e-007 1.593e-007 -6.750 -6.798 -0.047

H+ 2.620e-008 2.386e-008 -7.582 -7.622 -0.041

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 2.036e-006

H3BO3 1.994e-006 1.999e-006 -5.700 -5.699 0.001

H2BO3- 4.270e-008 3.837e-008 -7.370 -7.416 -0.046

Ba 7.796e-007

Ba+2 6.961e-007 4.586e-007 -6.157 -6.339 -0.181

BaSO4 5.971e-008 5.987e-008 -7.224 -7.223 0.001

BaHCO3+ 2.201e-008 1.978e-008 -7.657 -7.704 -0.046

BaCO3 1.807e-009 1.812e-009 -8.743 -8.742 0.001

BaOH+ 7.244e-013 6.510e-013 -12.140 -12.186 -0.046

C(4) 7.912e-003

HCO3- 7.279e-003 6.565e-003 -2.138 -2.183 -0.045

CO2 4.262e-004 4.273e-004 -3.370 -3.369 0.001

CaHCO3+ 1.193e-004 1.076e-004 -3.923 -3.968 -0.045

MgHCO3+ 4.496e-005 4.041e-005 -4.347 -4.394 -0.046

CaCO3 2.213e-005 2.219e-005 -4.655 -4.654 0.001

CO3-2 1.470e-005 9.731e-006 -4.833 -5.012 -0.179

MgCO3 4.208e-006 4.219e-006 -5.376 -5.375 0.001

NaHCO3 1.022e-006 1.025e-006 -5.990 -5.989 0.001

SrHCO3+ 4.551e-007 4.105e-007 -6.342 -6.387 -0.045

NaCO3- 2.979e-008 2.677e-008 -7.526 -7.572 -0.046

SrCO3 2.680e-008 2.687e-008 -7.572 -7.571 0.001

BaHCO3+ 2.201e-008 1.978e-008 -7.657 -7.704 -0.046

BaCO3 1.807e-009 1.812e-009 -8.743 -8.742 0.001

Ca 2.679e-003

Ca+2 2.462e-003 1.629e-003 -2.609 -2.788 -0.179

CaHCO3+ 1.193e-004 1.076e-004 -3.923 -3.968 -0.045

CaSO4 7.515e-005 7.534e-005 -4.124 -4.123 0.001

CaCO3 2.213e-005 2.219e-005 -4.655 -4.654 0.001

CaOH+ 1.260e-008 1.133e-008 -7.899 -7.946 -0.046

CaHSO4+ 1.027e-011 9.234e-012 -10.988 -11.035 -0.046

Cl 7.621e-005

Cl- 7.621e-005 6.835e-005 -4.118 -4.165 -0.047

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.742 -43.741 0.001

K 1.633e-005

K+ 1.630e-005 1.462e-005 -4.788 -4.835 -0.047

KSO4- 2.394e-008 2.152e-008 -7.621 -7.667 -0.046

KOH 2.119e-012 2.124e-012 -11.674 -11.673 0.001

Li 3.317e-006

Li+ 3.313e-006 2.994e-006 -5.480 -5.524 -0.044

LiSO4- 3.788e-009 3.404e-009 -8.422 -8.468 -0.046

LiOH 2.866e-012 2.873e-012 -11.543 -11.542 0.001

Mg 8.931e-004

Mg+2 8.198e-004 5.462e-004 -3.086 -3.263 -0.176

MgHCO3+ 4.496e-005 4.041e-005 -4.347 -4.394 -0.046

MgSO4 2.411e-005 2.417e-005 -4.618 -4.617 0.001

MgCO3 4.208e-006 4.219e-006 -5.376 -5.375 0.001

MgOH+ 2.990e-008 2.687e-008 -7.524 -7.571 -0.046

N(5) 1.929e-006

NO3- 1.929e-006 1.726e-006 -5.715 -5.763 -0.048

Na 3.099e-004

Na+ 3.085e-004 2.776e-004 -3.511 -3.557 -0.046

NaHCO3 1.022e-006 1.025e-006 -5.990 -5.989 0.001

NaSO4- 3.725e-007 3.348e-007 -6.429 -6.475 -0.046

NaCO3- 2.979e-008 2.677e-008 -7.526 -7.572 -0.046

NaOH 7.664e-011 7.684e-011 -10.116 -10.114 0.001

O(0) 2.321e-009

O2 1.160e-009 1.163e-009 -8.935 -8.934 0.001

S(6) 4.958e-004

SO4-2 3.958e-004 2.605e-004 -3.402 -3.584 -0.182

CaSO4 7.515e-005 7.534e-005 -4.124 -4.123 0.001

MgSO4 2.411e-005 2.417e-005 -4.618 -4.617 0.001

NaSO4- 3.725e-007 3.348e-007 -6.429 -6.475 -0.046

SrSO4 2.696e-007 2.703e-007 -6.569 -6.568 0.001

BaSO4 5.971e-008 5.987e-008 -7.224 -7.223 0.001

KSO4- 2.394e-008 2.152e-008 -7.621 -7.667 -0.046

LiSO4- 3.788e-009 3.404e-009 -8.422 -8.468 -0.046

HSO4- 5.246e-010 4.715e-010 -9.280 -9.327 -0.046

CaHSO4+ 1.027e-011 9.234e-012 -10.988 -11.035 -0.046

Si 8.077e-005

H4SiO4 8.042e-005 8.063e-005 -4.095 -4.094 0.001

H3SiO4- 3.528e-007 3.170e-007 -6.453 -6.499 -0.046

H2SiO4-2 5.983e-013 3.903e-013 -12.223 -12.409 -0.185

Sr 1.005e-005

Sr+2 9.298e-006 6.165e-006 -5.032 -5.210 -0.179

SrHCO3+ 4.551e-007 4.105e-007 -6.342 -6.387 -0.045

SrSO4 2.696e-007 2.703e-007 -6.569 -6.568 0.001

SrCO3 2.680e-008 2.687e-008 -7.572 -7.571 0.001

SrOH+ 1.470e-011 1.325e-011 -10.833 -10.878 -0.045

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.04 -6.37 -4.33 CaSO4

Aragonite 0.47 -7.80 -8.27 CaCO3

Barite 0.26 -9.92 -10.18 BaSO4

Calcite 0.62 -7.80 -8.42 CaCO3

Celestite -2.17 -8.79 -6.62 SrSO4

Chalcedony -0.40 -4.09 -3.70 SiO2

Chrysotile -5.99 27.76 33.75 Mg3Si2O5(OH)4

CO2(g) -2.06 -3.37 -1.31 CO2

Dolomite 0.73 -16.07 -16.80 CaMg(CO3)2

Gypsum -1.79 -6.37 -4.59 CaSO4:2H2O

H2(g) -40.64 -43.74 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.28 -7.72 1.55 NaCl

O2(g) -6.14 -8.93 -2.79 O2

Quartz 0.07 -4.09 -4.16 SiO2

Sepiolite -4.41 11.68 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -6.98 11.68 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.28 -4.09 -2.81 SiO2

Strontianite -0.94 -10.22 -9.28 SrCO3

Talc -3.25 19.57 22.82 Mg3Si4O10(OH)2

Witherite -2.74 -11.35 -8.61 BaCO3

Initial solution 2. 07-2-18

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 5.706e-003 5.706e-003

B 1.573e-006 1.573e-006

Ba 6.484e-007 6.484e-007

Ca 2.352e-003 2.352e-003

Cl 8.579e-005 8.579e-005

K 1.760e-005 1.760e-005

Li 3.028e-006 3.028e-006

Mg 8.148e-004 8.148e-004

Na 2.720e-004 2.720e-004

S(6) 4.728e-004 4.728e-004

Si 6.428e-005 6.428e-005

Sr 8.907e-006 8.907e-006

----------------------------Description of solution----------------------------

pH = 7.971 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 442

Density (g/cm3) = 0.99982

Activity of water = 1.000

Ionic strength = 9.653e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 5.784e-003

Total CO2 (mol/kg) = 5.784e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -9.313e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.74

Iterations = 9

Total H = 1.110183e+002

Total O = 5.552558e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.940e-007 3.559e-007 -6.404 -6.449 -0.044

H+ 1.166e-008 1.068e-008 -7.933 -7.971 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 1.573e-006

H3BO3 1.502e-006 1.505e-006 -5.823 -5.822 0.001

H2BO3- 7.132e-008 6.456e-008 -7.147 -7.190 -0.043

Ba 6.484e-007

Ba+2 5.807e-007 3.933e-007 -6.236 -6.405 -0.169

BaSO4 5.085e-008 5.097e-008 -7.294 -7.293 0.001

BaHCO3+ 1.416e-008 1.282e-008 -7.849 -7.892 -0.043

BaCO3 2.617e-009 2.623e-009 -8.582 -8.581 0.001

BaOH+ 1.378e-012 1.248e-012 -11.861 -11.904 -0.043

C(4) 5.784e-003

HCO3- 5.462e-003 4.960e-003 -2.263 -2.305 -0.042

CO2 1.442e-004 1.445e-004 -3.841 -3.840 0.001

CaHCO3+ 8.102e-005 7.358e-005 -4.091 -4.133 -0.042

CaCO3 3.382e-005 3.390e-005 -4.471 -4.470 0.001

MgHCO3+ 3.182e-005 2.881e-005 -4.497 -4.541 -0.043

CO3-2 2.415e-005 1.642e-005 -4.617 -4.785 -0.167

MgCO3 6.704e-006 6.719e-006 -5.174 -5.173 0.001

NaHCO3 6.833e-007 6.848e-007 -6.165 -6.164 0.001

SrHCO3+ 3.134e-007 2.846e-007 -6.504 -6.546 -0.042

NaCO3- 4.415e-008 3.997e-008 -7.355 -7.398 -0.043

SrCO3 4.152e-008 4.161e-008 -7.382 -7.381 0.001

BaHCO3+ 1.416e-008 1.282e-008 -7.849 -7.892 -0.043

BaCO3 2.617e-009 2.623e-009 -8.582 -8.581 0.001

Ca 2.352e-003

Ca+2 2.169e-003 1.475e-003 -2.664 -2.831 -0.168

CaHCO3+ 8.102e-005 7.358e-005 -4.091 -4.133 -0.042

CaSO4 6.753e-005 6.768e-005 -4.171 -4.170 0.001

CaCO3 3.382e-005 3.390e-005 -4.471 -4.470 0.001

CaOH+ 2.531e-008 2.291e-008 -7.597 -7.640 -0.043

CaHSO4+ 4.102e-012 3.713e-012 -11.387 -11.430 -0.043

Cl 8.579e-005

Cl- 8.579e-005 7.753e-005 -4.067 -4.111 -0.044

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -44.440 -44.439 0.001

K 1.760e-005

K+ 1.758e-005 1.589e-005 -4.755 -4.799 -0.044

KSO4- 2.563e-008 2.320e-008 -7.591 -7.634 -0.043

KOH 5.144e-012 5.156e-012 -11.289 -11.288 0.001

Li 3.028e-006

Li+ 3.025e-006 2.751e-006 -5.519 -5.561 -0.041

LiSO4- 3.430e-009 3.105e-009 -8.465 -8.508 -0.043

LiOH 5.886e-012 5.899e-012 -11.230 -11.229 0.001

Mg 8.148e-004

Mg+2 7.537e-004 5.154e-004 -3.123 -3.288 -0.165

MgHCO3+ 3.182e-005 2.881e-005 -4.497 -4.541 -0.043

MgSO4 2.259e-005 2.264e-005 -4.646 -4.645 0.001

MgCO3 6.704e-006 6.719e-006 -5.174 -5.173 0.001

MgOH+ 6.258e-008 5.664e-008 -7.204 -7.247 -0.043

Na 2.720e-004

Na+ 2.709e-004 2.455e-004 -3.567 -3.610 -0.043

NaHCO3 6.833e-007 6.848e-007 -6.165 -6.164 0.001

NaSO4- 3.247e-007 2.939e-007 -6.489 -6.532 -0.043

NaCO3- 4.415e-008 3.997e-008 -7.355 -7.398 -0.043

NaOH 1.515e-010 1.519e-010 -9.820 -9.819 0.001

O(0) 5.784e-008

O2 2.892e-008 2.899e-008 -7.539 -7.538 0.001

S(6) 4.728e-004

SO4-2 3.821e-004 2.585e-004 -3.418 -3.587 -0.170

CaSO4 6.753e-005 6.768e-005 -4.171 -4.170 0.001

MgSO4 2.259e-005 2.264e-005 -4.646 -4.645 0.001

NaSO4- 3.247e-007 2.939e-007 -6.489 -6.532 -0.043

SrSO4 2.456e-007 2.461e-007 -6.610 -6.609 0.001

BaSO4 5.085e-008 5.097e-008 -7.294 -7.293 0.001

KSO4- 2.563e-008 2.320e-008 -7.591 -7.634 -0.043

LiSO4- 3.430e-009 3.105e-009 -8.465 -8.508 -0.043

HSO4- 2.314e-010 2.094e-010 -9.636 -9.679 -0.043

CaHSO4+ 4.102e-012 3.713e-012 -11.387 -11.430 -0.043

Si 6.428e-005

H4SiO4 6.366e-005 6.380e-005 -4.196 -4.195 0.001

H3SiO4- 6.191e-007 5.604e-007 -6.208 -6.251 -0.043

H2SiO4-2 2.296e-012 1.542e-012 -11.639 -11.812 -0.173

Sr 8.907e-006

Sr+2 8.306e-006 5.657e-006 -5.081 -5.247 -0.167

SrHCO3+ 3.134e-007 2.846e-007 -6.504 -6.546 -0.042

SrSO4 2.456e-007 2.461e-007 -6.610 -6.609 0.001

SrCO3 4.152e-008 4.161e-008 -7.382 -7.381 0.001

SrOH+ 2.993e-011 2.716e-011 -10.524 -10.566 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.08 -6.42 -4.33 CaSO4

Aragonite 0.65 -7.62 -8.27 CaCO3

Barite 0.19 -9.99 -10.18 BaSO4

Calcite 0.81 -7.62 -8.42 CaCO3

Celestite -2.21 -8.83 -6.62 SrSO4

Chalcedony -0.50 -4.20 -3.70 SiO2

Chrysotile -4.17 29.57 33.75 Mg3Si2O5(OH)4

CO2(g) -2.53 -3.84 -1.31 CO2

Dolomite 1.11 -15.69 -16.80 CaMg(CO3)2

Gypsum -1.83 -6.42 -4.59 CaSO4:2H2O

H2(g) -41.34 -44.44 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.27 -7.72 1.55 NaCl

O2(g) -4.74 -7.54 -2.79 O2

Quartz -0.03 -4.20 -4.16 SiO2

Sepiolite -3.36 12.72 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -5.94 12.72 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.38 -4.20 -2.81 SiO2

Strontianite -0.75 -10.03 -9.28 SrCO3

Talc -1.64 21.18 22.82 Mg3Si4O10(OH)2

Witherite -2.58 -11.19 -8.61 BaCO3

Initial solution 3. 07-3-18

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 5.969e-003 5.969e-003

B 1.666e-006 1.666e-006

Ba 6.775e-007 6.775e-007

Ca 2.359e-003 2.359e-003

Cl 7.987e-005 7.987e-005

K 1.571e-005 1.571e-005

Li 2.884e-006 2.884e-006

Mg 8.395e-004 8.395e-004

N(5) 1.500e-006 1.500e-006

Na 2.829e-004 2.829e-004

S(6) 3.968e-004 3.968e-004

Si 7.377e-005 7.377e-005

Sr 9.021e-006 9.021e-006

----------------------------Description of solution----------------------------

pH = 7.956 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 446

Density (g/cm3) = 0.99982

Activity of water = 1.000

Ionic strength = 9.739e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.058e-003

Total CO2 (mol/kg) = 6.058e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -1.255e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.98

Iterations = 9

Total H = 1.110186e+002

Total O = 5.552613e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.802e-007 3.434e-007 -6.420 -6.464 -0.044

H+ 1.209e-008 1.107e-008 -7.918 -7.956 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 1.666e-006

H3BO3 1.593e-006 1.597e-006 -5.798 -5.797 0.001

H2BO3- 7.299e-008 6.605e-008 -7.137 -7.180 -0.043

Ba 6.775e-007

Ba+2 6.142e-007 4.153e-007 -6.212 -6.382 -0.170

BaSO4 4.491e-008 4.501e-008 -7.348 -7.347 0.001

BaHCO3+ 1.565e-008 1.416e-008 -7.806 -7.849 -0.043

BaCO3 2.788e-009 2.794e-009 -8.555 -8.554 0.001

BaOH+ 1.404e-012 1.271e-012 -11.852 -11.896 -0.043

C(4) 6.058e-003

HCO3- 5.715e-003 5.188e-003 -2.243 -2.285 -0.042

CO2 1.563e-004 1.567e-004 -3.806 -3.805 0.001

CaHCO3+ 8.519e-005 7.734e-005 -4.070 -4.112 -0.042

MgHCO3+ 3.436e-005 3.109e-005 -4.464 -4.507 -0.043

CaCO3 3.429e-005 3.437e-005 -4.465 -4.464 0.001

CO3-2 2.440e-005 1.657e-005 -4.613 -4.781 -0.168

MgCO3 6.979e-006 6.994e-006 -5.156 -5.155 0.001

NaHCO3 7.431e-007 7.448e-007 -6.129 -6.128 0.001

SrHCO3+ 3.326e-007 3.020e-007 -6.478 -6.520 -0.042

NaCO3- 4.634e-008 4.193e-008 -7.334 -7.377 -0.043

SrCO3 4.249e-008 4.259e-008 -7.372 -7.371 0.001

BaHCO3+ 1.565e-008 1.416e-008 -7.806 -7.849 -0.043

BaCO3 2.788e-009 2.794e-009 -8.555 -8.554 0.001

Ca 2.359e-003

Ca+2 2.183e-003 1.482e-003 -2.661 -2.829 -0.168

CaHCO3+ 8.519e-005 7.734e-005 -4.070 -4.112 -0.042

CaSO4 5.675e-005 5.688e-005 -4.246 -4.245 0.001

CaCO3 3.429e-005 3.437e-005 -4.465 -4.464 0.001

CaOH+ 2.454e-008 2.220e-008 -7.610 -7.654 -0.043

CaHSO4+ 3.575e-012 3.235e-012 -11.447 -11.490 -0.043

Cl 7.987e-005

Cl- 7.987e-005 7.214e-005 -4.098 -4.142 -0.044

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -44.408 -44.407 0.001

K 1.571e-005

K+ 1.569e-005 1.417e-005 -4.804 -4.848 -0.044

KSO4- 1.913e-008 1.731e-008 -7.718 -7.762 -0.043

KOH 4.428e-012 4.438e-012 -11.354 -11.353 0.001

Li 2.884e-006

Li+ 2.881e-006 2.620e-006 -5.540 -5.582 -0.041

LiSO4- 2.733e-009 2.473e-009 -8.563 -8.607 -0.043

LiOH 5.407e-012 5.419e-012 -11.267 -11.266 0.001

Mg 8.395e-004

Mg+2 7.787e-004 5.318e-004 -3.109 -3.274 -0.166

MgHCO3+ 3.436e-005 3.109e-005 -4.464 -4.507 -0.043

MgSO4 1.949e-005 1.953e-005 -4.710 -4.709 0.001

MgCO3 6.979e-006 6.994e-006 -5.156 -5.155 0.001

MgOH+ 6.230e-008 5.637e-008 -7.206 -7.249 -0.043

N(5) 1.500e-006

NO3- 1.500e-006 1.353e-006 -5.824 -5.869 -0.045

Na 2.829e-004

Na+ 2.818e-004 2.553e-004 -3.550 -3.593 -0.043

NaHCO3 7.431e-007 7.448e-007 -6.129 -6.128 0.001

NaSO4- 2.824e-007 2.556e-007 -6.549 -6.593 -0.043

NaCO3- 4.634e-008 4.193e-008 -7.334 -7.377 -0.043

NaOH 1.520e-010 1.523e-010 -9.818 -9.817 0.001

O(0) 5.008e-008

O2 2.504e-008 2.510e-008 -7.601 -7.600 0.001

S(6) 3.968e-004

SO4-2 3.200e-004 2.162e-004 -3.495 -3.665 -0.170

CaSO4 5.675e-005 5.688e-005 -4.246 -4.245 0.001

MgSO4 1.949e-005 1.953e-005 -4.710 -4.709 0.001

NaSO4- 2.824e-007 2.556e-007 -6.549 -6.593 -0.043

SrSO4 2.083e-007 2.088e-007 -6.681 -6.680 0.001

BaSO4 4.491e-008 4.501e-008 -7.348 -7.347 0.001

KSO4- 1.913e-008 1.731e-008 -7.718 -7.762 -0.043

LiSO4- 2.733e-009 2.473e-009 -8.563 -8.607 -0.043

HSO4- 2.007e-010 1.816e-010 -9.697 -9.741 -0.043

CaHSO4+ 3.575e-012 3.235e-012 -11.447 -11.490 -0.043

Si 7.377e-005

H4SiO4 7.308e-005 7.325e-005 -4.136 -4.135 0.001

H3SiO4- 6.859e-007 6.207e-007 -6.164 -6.207 -0.043

H2SiO4-2 2.457e-012 1.647e-012 -11.610 -11.783 -0.174

Sr 9.021e-006

Sr+2 8.438e-006 5.738e-006 -5.074 -5.241 -0.167

SrHCO3+ 3.326e-007 3.020e-007 -6.478 -6.520 -0.042

SrSO4 2.083e-007 2.088e-007 -6.681 -6.680 0.001

SrCO3 4.249e-008 4.259e-008 -7.372 -7.371 0.001

SrOH+ 2.930e-011 2.657e-011 -10.533 -10.576 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.16 -6.49 -4.33 CaSO4

Aragonite 0.66 -7.61 -8.27 CaCO3

Barite 0.14 -10.05 -10.18 BaSO4

Calcite 0.81 -7.61 -8.42 CaCO3

Celestite -2.28 -8.91 -6.62 SrSO4

Chalcedony -0.44 -4.14 -3.70 SiO2

Chrysotile -4.11 29.64 33.75 Mg3Si2O5(OH)4

CO2(g) -2.49 -3.80 -1.31 CO2

Dolomite 1.14 -15.66 -16.80 CaMg(CO3)2

Gypsum -1.91 -6.49 -4.59 CaSO4:2H2O

H2(g) -41.31 -44.41 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.29 -7.73 1.55 NaCl

O2(g) -4.81 -7.60 -2.79 O2

Quartz 0.03 -4.14 -4.16 SiO2

Sepiolite -3.22 12.87 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -5.79 12.87 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.32 -4.14 -2.81 SiO2

Strontianite -0.74 -10.02 -9.28 SrCO3

Talc -1.45 21.37 22.82 Mg3Si4O10(OH)2

Witherite -2.55 -11.16 -8.61 BaCO3

Initial solution 4. 07-4-22

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 1.598e-005 1.598e-005

Alkalinity 5.886e-003 5.886e-003

B 2.592e-006 2.592e-006

Ba 7.503e-007 7.503e-007

Ca 2.302e-003 2.302e-003

Cl 7.704e-005 7.704e-005

K 1.973e-005 1.973e-005

Li 3.749e-006 3.749e-006

Mg 7.942e-004 7.942e-004

N(5) 1.143e-006 1.143e-006

Na 1.941e-004 1.941e-004

S(6) 2.041e-004 2.041e-004

Si 1.009e-004 1.009e-004

Sr 9.592e-006 9.592e-006

----------------------------Description of solution----------------------------

pH = 7.887 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 420

Density (g/cm3) = 0.99979

Activity of water = 1.000

Ionic strength = 9.214e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 5.947e-003

Total CO2 (mol/kg) = 5.947e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = 1.050e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.86

Iterations = 11

Total H = 1.110186e+002

Total O = 5.552517e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.234e-007 2.928e-007 -6.490 -6.533 -0.043

H+ 1.415e-008 1.298e-008 -7.849 -7.887 -0.037

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 1.598e-005

Al(OH)4- 1.584e-005 1.437e-005 -4.800 -4.843 -0.042

Al(OH)3 1.114e-007 1.116e-007 -6.953 -6.952 0.001

Al(OH)2+ 2.831e-008 2.568e-008 -7.548 -7.590 -0.042

AlOH+2 1.939e-010 1.312e-010 -9.712 -9.882 -0.170

Al+3 8.300e-013 3.823e-013 -12.081 -12.418 -0.337

AlSO4+ 1.273e-013 1.154e-013 -12.895 -12.938 -0.042

Al(SO4)2- 4.264e-016 3.868e-016 -15.370 -15.413 -0.042

AlHSO4+2 1.801e-022 1.219e-022 -21.744 -21.914 -0.170

B 2.592e-006

H3BO3 2.494e-006 2.500e-006 -5.603 -5.602 0.001

H2BO3- 9.721e-008 8.817e-008 -7.012 -7.055 -0.042

Ba 7.503e-007

Ba+2 7.030e-007 4.798e-007 -6.153 -6.319 -0.166

BaSO4 2.695e-008 2.700e-008 -7.569 -7.569 0.001

BaHCO3+ 1.770e-008 1.605e-008 -7.752 -7.795 -0.042

BaCO3 2.696e-009 2.701e-009 -8.569 -8.568 0.001

BaOH+ 1.380e-012 1.252e-012 -11.860 -11.902 -0.042

C(4) 5.947e-003

HCO3- 5.595e-003 5.091e-003 -2.252 -2.293 -0.041

CO2 1.799e-004 1.803e-004 -3.745 -3.744 0.001

CaHCO3+ 8.329e-005 7.579e-005 -4.079 -4.120 -0.041

MgHCO3+ 3.252e-005 2.949e-005 -4.488 -4.530 -0.042

CaCO3 2.866e-005 2.872e-005 -4.543 -4.542 0.001

CO3-2 2.023e-005 1.387e-005 -4.694 -4.858 -0.164

MgCO3 5.646e-006 5.658e-006 -5.248 -5.247 0.001

NaHCO3 5.018e-007 5.029e-007 -6.299 -6.299 0.001

SrHCO3+ 3.537e-007 3.218e-007 -6.451 -6.492 -0.041

SrCO3 3.862e-008 3.870e-008 -7.413 -7.412 0.001

NaCO3- 2.662e-008 2.414e-008 -7.575 -7.617 -0.042

BaHCO3+ 1.770e-008 1.605e-008 -7.752 -7.795 -0.042

BaCO3 2.696e-009 2.701e-009 -8.569 -8.568 0.001

Ca 2.302e-003

Ca+2 2.160e-003 1.480e-003 -2.666 -2.830 -0.164

CaHCO3+ 8.329e-005 7.579e-005 -4.079 -4.120 -0.041

CaSO4 2.943e-005 2.950e-005 -4.531 -4.530 0.001

CaCO3 2.866e-005 2.872e-005 -4.543 -4.542 0.001

CaOH+ 2.085e-008 1.891e-008 -7.681 -7.723 -0.042

CaHSO4+ 2.169e-012 1.967e-012 -11.664 -11.706 -0.042

Cl 7.704e-005

Cl- 7.704e-005 6.977e-005 -4.113 -4.156 -0.043

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -44.270 -44.269 0.001

K 1.973e-005

K+ 1.972e-005 1.785e-005 -4.705 -4.748 -0.043

KSO4- 1.249e-008 1.133e-008 -7.904 -7.946 -0.042

KOH 4.756e-012 4.767e-012 -11.323 -11.322 0.001

Li 3.749e-006

Li+ 3.747e-006 3.414e-006 -5.426 -5.467 -0.040

LiSO4- 1.845e-009 1.674e-009 -8.734 -8.776 -0.042

LiOH 6.010e-012 6.023e-012 -11.221 -11.220 0.001

Mg 7.942e-004

Mg+2 7.462e-004 5.141e-004 -3.127 -3.289 -0.162

MgHCO3+ 3.252e-005 2.949e-005 -4.488 -4.530 -0.042

MgSO4 9.787e-006 9.807e-006 -5.009 -5.008 0.001

MgCO3 5.646e-006 5.658e-006 -5.248 -5.247 0.001

MgOH+ 5.124e-008 4.648e-008 -7.290 -7.333 -0.042

N(5) 1.143e-006

NO3- 1.143e-006 1.033e-006 -5.942 -5.986 -0.044

Na 1.941e-004

Na+ 1.935e-004 1.757e-004 -3.713 -3.755 -0.042

NaHCO3 5.018e-007 5.029e-007 -6.299 -6.299 0.001

NaSO4- 1.007e-007 9.132e-008 -6.997 -7.039 -0.042

NaCO3- 2.662e-008 2.414e-008 -7.575 -7.617 -0.042

NaOH 8.918e-011 8.937e-011 -10.050 -10.049 0.001

O(0) 2.648e-008

O2 1.324e-008 1.327e-008 -7.878 -7.877 0.001

S(6) 2.041e-004

SO4-2 1.647e-004 1.123e-004 -3.783 -3.950 -0.166

CaSO4 2.943e-005 2.950e-005 -4.531 -4.530 0.001

MgSO4 9.787e-006 9.807e-006 -5.009 -5.008 0.001

SrSO4 1.175e-007 1.178e-007 -6.930 -6.929 0.001

NaSO4- 1.007e-007 9.132e-008 -6.997 -7.039 -0.042

BaSO4 2.695e-008 2.700e-008 -7.569 -7.569 0.001

KSO4- 1.249e-008 1.133e-008 -7.904 -7.946 -0.042

LiSO4- 1.845e-009 1.674e-009 -8.734 -8.776 -0.042

HSO4- 1.219e-010 1.106e-010 -9.914 -9.956 -0.042

CaHSO4+ 2.169e-012 1.967e-012 -11.664 -11.706 -0.042

AlSO4+ 1.273e-013 1.154e-013 -12.895 -12.938 -0.042

Al(SO4)2- 4.264e-016 3.868e-016 -15.370 -15.413 -0.042

AlHSO4+2 1.801e-022 1.219e-022 -21.744 -21.914 -0.170

Si 1.009e-004

H4SiO4 1.001e-004 1.003e-004 -4.000 -3.999 0.001

H3SiO4- 7.992e-007 7.249e-007 -6.097 -6.140 -0.042

H2SiO4-2 2.423e-012 1.640e-012 -11.616 -11.785 -0.170

Sr 9.592e-006

Sr+2 9.082e-006 6.231e-006 -5.042 -5.205 -0.164

SrHCO3+ 3.537e-007 3.218e-007 -6.451 -6.492 -0.041

SrSO4 1.175e-007 1.178e-007 -6.930 -6.929 0.001

SrCO3 3.862e-008 3.870e-008 -7.413 -7.412 0.001

SrOH+ 2.707e-011 2.461e-011 -10.567 -10.609 -0.041

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -0.37 11.24 11.61 Al(OH)3

Albite -1.80 -20.59 -18.80 NaAlSi3O8

Alunite -2.73 -2.58 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.45 -6.78 -4.33 CaSO4

Anorthite -0.44 -20.51 -20.07 CaAl2Si2O8

Aragonite 0.58 -7.69 -8.27 CaCO3

Barite -0.08 -10.27 -10.18 BaSO4

Ca-Montmorillonite 4.62 -42.20 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.73 -7.69 -8.42 CaCO3

Celestite -2.53 -9.16 -6.62 SrSO4

Chalcedony -0.30 -4.00 -3.70 SiO2

Chlorite(14A) -0.13 72.91 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -4.29 29.46 33.75 Mg3Si2O5(OH)4

CO2(g) -2.43 -3.74 -1.31 CO2

Dolomite 0.97 -15.83 -16.80 CaMg(CO3)2

Gibbsite 2.43 11.24 8.81 Al(OH)3

Gypsum -2.19 -6.78 -4.59 CaSO4:2H2O

H2(g) -41.17 -44.27 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.47 -7.91 1.55 NaCl

Illite 3.68 -38.27 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -0.07 -21.59 -21.52 KAlSi3O8

K-mica 10.34 24.87 14.53 KAl3Si3O10(OH)2

Kaolinite 5.97 14.49 8.52 Al2Si2O5(OH)4

O2(g) -5.08 -7.88 -2.79 O2

Quartz 0.17 -4.00 -4.16 SiO2

Sepiolite -3.12 12.97 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -5.69 12.97 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.18 -4.00 -2.81 SiO2

Strontianite -0.78 -10.06 -9.28 SrCO3

Talc -1.37 21.46 22.82 Mg3Si4O10(OH)2

Witherite -2.57 -11.18 -8.61 BaCO3

Initial solution 5. 07-6-4

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 3.708e-008 3.708e-008

Alkalinity 5.821e-003 5.821e-003

B 2.962e-006 2.962e-006

Ba 7.430e-007 7.430e-007

Ca 2.157e-003 2.157e-003

Cl 6.011e-005 6.011e-005

K 1.950e-005 1.950e-005

Li 3.749e-006 3.749e-006

Mg 7.366e-004 7.366e-004

N(5) 1.429e-006 1.429e-006

Na 1.880e-004 1.880e-004

S(6) 1.479e-004 1.479e-004

Si 9.458e-005 9.458e-005

Sr 9.135e-006 9.135e-006

----------------------------Description of solution----------------------------

pH = 7.731 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 404

Density (g/cm3) = 0.99978

Activity of water = 1.000

Ionic strength = 8.762e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.043e-003

Total CO2 (mol/kg) = 6.043e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -1.602e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.36

Iterations = 10

Total H = 1.110186e+002

Total O = 5.552507e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.254e-007 2.045e-007 -6.647 -6.689 -0.042

H+ 2.023e-008 1.859e-008 -7.694 -7.731 -0.037

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 3.708e-008

Al(OH)4- 3.658e-008 3.325e-008 -7.437 -7.478 -0.041

Al(OH)3 3.691e-010 3.699e-010 -9.433 -9.432 0.001

Al(OH)2+ 1.340e-010 1.218e-010 -9.873 -9.914 -0.041

AlOH+2 1.306e-012 8.914e-013 -11.884 -12.050 -0.166

Al+3 7.952e-015 3.718e-015 -14.100 -14.430 -0.330

AlSO4+ 9.100e-016 8.272e-016 -15.041 -15.082 -0.041

Al(SO4)2- 2.247e-018 2.042e-018 -17.648 -17.690 -0.041

AlHSO4+2 1.833e-024 1.251e-024 -23.737 -23.903 -0.166

B 2.962e-006

H3BO3 2.883e-006 2.889e-006 -5.540 -5.539 0.001

H2BO3- 7.830e-008 7.117e-008 -7.106 -7.148 -0.041

Ba 7.430e-007

Ba+2 7.031e-007 4.839e-007 -6.153 -6.315 -0.162

BaSO4 2.002e-008 2.006e-008 -7.698 -7.698 0.001

BaHCO3+ 1.797e-008 1.633e-008 -7.746 -7.787 -0.041

BaCO3 1.916e-009 1.920e-009 -8.718 -8.717 0.001

BaOH+ 9.700e-013 8.817e-013 -12.013 -12.055 -0.041

C(4) 6.043e-003

HCO3- 5.634e-003 5.137e-003 -2.249 -2.289 -0.040

CO2 2.599e-004 2.605e-004 -3.585 -3.584 0.001

CaHCO3+ 7.973e-005 7.269e-005 -4.098 -4.139 -0.040

MgHCO3+ 3.074e-005 2.794e-005 -4.512 -4.554 -0.041

CaCO3 1.920e-005 1.924e-005 -4.717 -4.716 0.001

CO3-2 1.414e-005 9.771e-006 -4.849 -5.010 -0.161

MgCO3 3.736e-006 3.744e-006 -5.428 -5.427 0.001

NaHCO3 4.916e-007 4.926e-007 -6.308 -6.308 0.001

SrHCO3+ 3.432e-007 3.129e-007 -6.464 -6.505 -0.040

SrCO3 2.622e-008 2.628e-008 -7.581 -7.580 0.001

NaCO3- 1.817e-008 1.651e-008 -7.741 -7.782 -0.041

BaHCO3+ 1.797e-008 1.633e-008 -7.746 -7.787 -0.041

BaCO3 1.916e-009 1.920e-009 -8.718 -8.717 0.001

Ca 2.157e-003

Ca+2 2.037e-003 1.407e-003 -2.691 -2.852 -0.161

CaHCO3+ 7.973e-005 7.269e-005 -4.098 -4.139 -0.040

CaSO4 2.062e-005 2.066e-005 -4.686 -4.685 0.001

CaCO3 1.920e-005 1.924e-005 -4.717 -4.716 0.001

CaOH+ 1.381e-008 1.255e-008 -7.860 -7.901 -0.041

CaHSO4+ 2.171e-012 1.973e-012 -11.663 -11.705 -0.041

Cl 6.011e-005

Cl- 6.011e-005 5.455e-005 -4.221 -4.263 -0.042

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.958 -43.957 0.001

K 1.950e-005

K+ 1.949e-005 1.769e-005 -4.710 -4.752 -0.042

KSO4- 9.094e-009 8.266e-009 -8.041 -8.083 -0.041

KOH 3.291e-012 3.298e-012 -11.483 -11.482 0.001

Li 3.749e-006

Li+ 3.747e-006 3.421e-006 -5.426 -5.466 -0.040

LiSO4- 1.359e-009 1.236e-009 -8.867 -8.908 -0.041

LiOH 4.206e-012 4.215e-012 -11.376 -11.375 0.001

Mg 7.366e-004

Mg+2 6.953e-004 4.828e-004 -3.158 -3.316 -0.158

MgHCO3+ 3.074e-005 2.794e-005 -4.512 -4.554 -0.041

MgSO4 6.772e-006 6.786e-006 -5.169 -5.168 0.001

MgCO3 3.736e-006 3.744e-006 -5.428 -5.427 0.001

MgOH+ 3.353e-008 3.048e-008 -7.475 -7.516 -0.041

N(5) 1.429e-006

NO3- 1.429e-006 1.294e-006 -5.845 -5.888 -0.043

Na 1.880e-004

Na+ 1.874e-004 1.705e-004 -3.727 -3.768 -0.041

NaHCO3 4.916e-007 4.926e-007 -6.308 -6.308 0.001

NaSO4- 7.186e-008 6.532e-008 -7.144 -7.185 -0.041

NaCO3- 1.817e-008 1.651e-008 -7.741 -7.782 -0.041

NaOH 6.046e-011 6.059e-011 -10.219 -10.218 0.001

O(0) 6.301e-009

O2 3.150e-009 3.157e-009 -8.502 -8.501 0.001

S(6) 1.479e-004

SO4-2 1.203e-004 8.273e-005 -3.920 -4.082 -0.163

CaSO4 2.062e-005 2.066e-005 -4.686 -4.685 0.001

MgSO4 6.772e-006 6.786e-006 -5.169 -5.168 0.001

SrSO4 8.344e-008 8.360e-008 -7.079 -7.078 0.001

NaSO4- 7.186e-008 6.532e-008 -7.144 -7.185 -0.041

BaSO4 2.002e-008 2.006e-008 -7.698 -7.698 0.001

KSO4- 9.094e-009 8.266e-009 -8.041 -8.083 -0.041

LiSO4- 1.359e-009 1.236e-009 -8.867 -8.908 -0.041

HSO4- 1.284e-010 1.167e-010 -9.892 -9.933 -0.041

CaHSO4+ 2.171e-012 1.973e-012 -11.663 -11.705 -0.041

AlSO4+ 9.100e-016 8.272e-016 -15.041 -15.082 -0.041

Al(SO4)2- 2.247e-018 2.042e-018 -17.648 -17.690 -0.041

AlHSO4+2 1.833e-024 1.251e-024 -23.737 -23.903 -0.166

Si 9.458e-005

H4SiO4 9.406e-005 9.425e-005 -4.027 -4.026 0.001

H3SiO4- 5.232e-007 4.756e-007 -6.281 -6.323 -0.041

H2SiO4-2 1.101e-012 7.515e-013 -11.958 -12.124 -0.166

Sr 9.135e-006

Sr+2 8.682e-006 6.005e-006 -5.061 -5.222 -0.160

SrHCO3+ 3.432e-007 3.129e-007 -6.464 -6.505 -0.040

SrSO4 8.344e-008 8.360e-008 -7.079 -7.078 0.001

SrCO3 2.622e-008 2.628e-008 -7.581 -7.580 0.001

SrOH+ 1.818e-011 1.656e-011 -10.740 -10.781 -0.041

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -2.85 8.76 11.61 Al(OH)3

Albite -4.53 -23.32 -18.80 NaAlSi3O8

Alunite -9.97 -9.82 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.60 -6.93 -4.33 CaSO4

Anorthite -5.79 -25.86 -20.07 CaAl2Si2O8

Aragonite 0.41 -7.86 -8.27 CaCO3

Barite -0.21 -10.40 -10.18 BaSO4

Ca-Montmorillonite -1.31 -48.13 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.56 -7.86 -8.42 CaCO3

Celestite -2.68 -9.30 -6.62 SrSO4

Chalcedony -0.33 -4.03 -3.70 SiO2

Chlorite(14A) -6.86 66.17 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -5.36 28.38 33.75 Mg3Si2O5(OH)4

CO2(g) -2.27 -3.58 -1.31 CO2

Dolomite 0.61 -16.19 -16.80 CaMg(CO3)2

Gibbsite -0.05 8.76 8.81 Al(OH)3

Gypsum -2.35 -6.93 -4.59 CaSO4:2H2O

H2(g) -40.86 -43.96 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.59 -8.03 1.55 NaCl

Illite -2.30 -44.25 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -2.79 -24.31 -21.52 KAlSi3O8

K-mica 2.66 17.19 14.53 KAl3Si3O10(OH)2

Kaolinite 0.95 9.47 8.52 Al2Si2O5(OH)4

O2(g) -5.71 -8.50 -2.79 O2

Quartz 0.14 -4.03 -4.16 SiO2

Sepiolite -3.88 12.21 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -6.45 12.21 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.21 -4.03 -2.81 SiO2

Strontianite -0.95 -10.23 -9.28 SrCO3

Talc -2.49 20.33 22.82 Mg3Si4O10(OH)2

Witherite -2.72 -11.33 -8.61 BaCO3

Initial solution 6. 07-7-24

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 3.338e-007 3.338e-007

Alkalinity 6.739e-003 6.739e-003

B 3.888e-006 3.888e-006

Ba 8.961e-007 8.961e-007

Ca 2.489e-003 2.489e-003

Cl 7.084e-005 7.084e-005

K 2.423e-005 2.423e-005

Li 4.182e-006 4.182e-006

Mg 8.066e-004 8.066e-004

Na 2.037e-004 2.037e-004

S(6) 2.521e-004 2.521e-004

Si 1.074e-004 1.074e-004

Sr 1.051e-005 1.051e-005

----------------------------Description of solution----------------------------

pH = 7.389 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 465

Density (g/cm3) = 0.99984

Activity of water = 1.000

Ionic strength = 1.012e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.376e-003

Total CO2 (mol/kg) = 7.376e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -4.673e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.43

Iterations = 11

Total H = 1.110196e+002

Total O = 5.552914e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.034e-007 9.319e-008 -6.986 -7.031 -0.045

H+ 4.461e-008 4.080e-008 -7.351 -7.389 -0.039

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 3.338e-007

Al(OH)4- 3.209e-007 2.899e-007 -6.494 -6.538 -0.044

Al(OH)3 7.060e-009 7.077e-009 -8.151 -8.150 0.001

Al(OH)2+ 5.660e-009 5.113e-009 -8.247 -8.291 -0.044

AlOH+2 1.233e-010 8.211e-011 -9.909 -10.086 -0.177

Al+3 1.679e-012 7.515e-013 -11.775 -12.124 -0.349

AlSO4+ 3.035e-013 2.741e-013 -12.518 -12.562 -0.044

Al(SO4)2- 1.228e-015 1.110e-015 -14.911 -14.955 -0.044

AlHSO4+2 1.366e-021 9.097e-022 -20.864 -21.041 -0.177

B 3.888e-006

H3BO3 3.840e-006 3.849e-006 -5.416 -5.415 0.001

H2BO3- 4.784e-008 4.321e-008 -7.320 -7.364 -0.044

Ba 8.961e-007

Ba+2 8.328e-007 5.595e-007 -6.079 -6.252 -0.173

BaSO4 3.795e-008 3.804e-008 -7.421 -7.420 0.001

BaHCO3+ 2.417e-008 2.183e-008 -7.617 -7.661 -0.044

BaCO3 1.167e-009 1.170e-009 -8.933 -8.932 0.001

BaOH+ 5.144e-013 4.647e-013 -12.289 -12.333 -0.044

C(4) 7.376e-003

HCO3- 6.553e-003 5.939e-003 -2.184 -2.226 -0.043

CO2 6.593e-004 6.608e-004 -3.181 -3.180 0.001

CaHCO3+ 1.039e-004 9.414e-005 -3.984 -4.026 -0.043

MgHCO3+ 3.795e-005 3.428e-005 -4.421 -4.465 -0.044

CaCO3 1.133e-005 1.136e-005 -4.946 -4.945 0.001

CO3-2 7.630e-006 5.149e-006 -5.117 -5.288 -0.171

MgCO3 2.089e-006 2.094e-006 -5.680 -5.679 0.001

NaHCO3 6.115e-007 6.129e-007 -6.214 -6.213 0.001

SrHCO3+ 4.444e-007 4.028e-007 -6.352 -6.395 -0.043

BaHCO3+ 2.417e-008 2.183e-008 -7.617 -7.661 -0.044

SrCO3 1.538e-008 1.542e-008 -7.813 -7.812 0.001

NaCO3- 1.037e-008 9.365e-009 -7.984 -8.028 -0.044

BaCO3 1.167e-009 1.170e-009 -8.933 -8.932 0.001

Ca 2.489e-003

Ca+2 2.336e-003 1.575e-003 -2.632 -2.803 -0.171

CaHCO3+ 1.039e-004 9.414e-005 -3.984 -4.026 -0.043

CaSO4 3.785e-005 3.794e-005 -4.422 -4.421 0.001

CaCO3 1.133e-005 1.136e-005 -4.946 -4.945 0.001

CaOH+ 7.094e-009 6.408e-009 -8.149 -8.193 -0.044

CaHSO4+ 8.801e-012 7.950e-012 -11.055 -11.100 -0.044

Cl 7.084e-005

Cl- 7.084e-005 6.388e-005 -4.150 -4.195 -0.045

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.276 -43.275 0.001

K 2.423e-005

K+ 2.421e-005 2.183e-005 -4.616 -4.661 -0.045

KSO4- 1.852e-008 1.673e-008 -7.732 -7.776 -0.044

KOH 1.851e-012 1.855e-012 -11.733 -11.732 0.001

Li 4.182e-006

Li+ 4.179e-006 3.794e-006 -5.379 -5.421 -0.042

LiSO4- 2.487e-009 2.247e-009 -8.604 -8.648 -0.044

LiOH 2.125e-012 2.130e-012 -11.673 -11.672 0.001

Mg 8.066e-004

Mg+2 7.548e-004 5.123e-004 -3.122 -3.290 -0.168

MgHCO3+ 3.795e-005 3.428e-005 -4.421 -4.465 -0.044

MgSO4 1.178e-005 1.181e-005 -4.929 -4.928 0.001

MgCO3 2.089e-006 2.094e-006 -5.680 -5.679 0.001

MgOH+ 1.632e-008 1.474e-008 -7.787 -7.831 -0.044

Na 2.037e-004

Na+ 2.029e-004 1.835e-004 -3.693 -3.736 -0.044

NaHCO3 6.115e-007 6.129e-007 -6.214 -6.213 0.001

NaSO4- 1.276e-007 1.153e-007 -6.894 -6.938 -0.044

NaCO3- 1.037e-008 9.365e-009 -7.984 -8.028 -0.044

NaOH 2.965e-011 2.972e-011 -10.528 -10.527 0.001

O(0) 2.717e-010

O2 1.359e-010 1.362e-010 -9.867 -9.866 0.001

S(6) 2.521e-004

SO4-2 2.021e-004 1.356e-004 -3.694 -3.868 -0.173

CaSO4 3.785e-005 3.794e-005 -4.422 -4.421 0.001

MgSO4 1.178e-005 1.181e-005 -4.929 -4.928 0.001

SrSO4 1.523e-007 1.526e-007 -6.817 -6.816 0.001

NaSO4- 1.276e-007 1.153e-007 -6.894 -6.938 -0.044

BaSO4 3.795e-008 3.804e-008 -7.421 -7.420 0.001

KSO4- 1.852e-008 1.673e-008 -7.732 -7.776 -0.044

LiSO4- 2.487e-009 2.247e-009 -8.604 -8.648 -0.044

HSO4- 4.647e-010 4.197e-010 -9.333 -9.377 -0.044

CaHSO4+ 8.801e-012 7.950e-012 -11.055 -11.100 -0.044

AlSO4+ 3.035e-013 2.741e-013 -12.518 -12.562 -0.044

Al(SO4)2- 1.228e-015 1.110e-015 -14.911 -14.955 -0.044

AlHSO4+2 1.366e-021 9.097e-022 -20.864 -21.041 -0.177

Si 1.074e-004

H4SiO4 1.071e-004 1.074e-004 -3.970 -3.969 0.001

H3SiO4- 2.734e-007 2.470e-007 -6.563 -6.607 -0.044

H2SiO4-2 2.671e-013 1.779e-013 -12.573 -12.750 -0.177

Sr 1.051e-005

Sr+2 9.894e-006 6.685e-006 -5.005 -5.175 -0.170

SrHCO3+ 4.444e-007 4.028e-007 -6.352 -6.395 -0.043

SrSO4 1.523e-007 1.526e-007 -6.817 -6.816 0.001

SrCO3 1.538e-008 1.542e-008 -7.813 -7.812 0.001

SrOH+ 9.281e-012 8.403e-012 -11.032 -11.076 -0.043

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -1.57 10.04 11.61 Al(OH)3

Albite -3.38 -22.18 -18.80 NaAlSi3O8

Alunite -4.58 -4.43 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.34 -6.67 -4.33 CaSO4

Anorthite -3.75 -23.82 -20.07 CaAl2Si2O8

Aragonite 0.18 -8.09 -8.27 CaCO3

Barite 0.06 -10.12 -10.18 BaSO4

Ca-Montmorillonite 1.78 -45.04 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.33 -8.09 -8.42 CaCO3

Celestite -2.42 -9.04 -6.62 SrSO4

Chalcedony -0.27 -3.97 -3.70 SiO2

Chlorite(14A) -7.41 65.62 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -7.22 26.53 33.75 Mg3Si2O5(OH)4

CO2(g) -1.87 -3.18 -1.31 CO2

Dolomite 0.13 -16.67 -16.80 CaMg(CO3)2

Gibbsite 1.23 10.04 8.81 Al(OH)3

Gypsum -2.08 -6.67 -4.59 CaSO4:2H2O

H2(g) -40.18 -43.27 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.48 -7.93 1.55 NaCl

Illite 0.53 -41.41 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -1.58 -23.11 -21.52 KAlSi3O8

K-mica 6.43 20.95 14.53 KAl3Si3O10(OH)2

Kaolinite 3.63 12.15 8.52 Al2Si2O5(OH)4

O2(g) -7.07 -9.87 -2.79 O2

Quartz 0.20 -3.97 -4.16 SiO2

Sepiolite -5.02 11.07 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -7.59 11.07 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.15 -3.97 -2.81 SiO2

Strontianite -1.18 -10.46 -9.28 SrCO3

Talc -4.23 18.59 22.82 Mg3Si4O10(OH)2

Witherite -2.93 -11.54 -8.61 BaCO3

Initial solution 7. 07-8-26

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 5.886e-003 5.886e-003

B 3.332e-006 3.332e-006

Ba 3.934e-007 3.934e-007

Ca 2.044e-003 2.044e-003

Cl 8.805e-005 8.805e-005

K 2.984e-005 2.984e-005

Li 4.614e-006 4.614e-006

Mg 1.078e-003 1.078e-003

N(5) 1.929e-006 1.929e-006

Na 2.559e-004 2.559e-004

S(6) 4.052e-004 4.052e-004

Si 9.475e-005 9.475e-005

Sr 1.736e-005 1.736e-005

----------------------------Description of solution----------------------------

pH = 7.413 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 441

Density (g/cm3) = 0.99981

Activity of water = 1.000

Ionic strength = 9.647e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.415e-003

Total CO2 (mol/kg) = 6.415e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -2.155e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.69

Iterations = 9

Total H = 1.110187e+002

Total O = 5.552693e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.089e-007 9.836e-008 -6.963 -7.007 -0.044

H+ 4.219e-008 3.865e-008 -7.375 -7.413 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 3.332e-006

H3BO3 3.289e-006 3.296e-006 -5.483 -5.482 0.001

H2BO3- 4.315e-008 3.906e-008 -7.365 -7.408 -0.043

Ba 3.934e-007

Ba+2 3.570e-007 2.418e-007 -6.447 -6.617 -0.169

BaSO4 2.681e-008 2.687e-008 -7.572 -7.571 0.001

BaHCO3+ 9.131e-009 8.266e-009 -8.039 -8.083 -0.043

BaCO3 4.663e-010 4.674e-010 -9.331 -9.330 0.001

BaOH+ 2.341e-013 2.119e-013 -12.631 -12.674 -0.043

C(4) 6.415e-003

HCO3- 5.729e-003 5.203e-003 -2.242 -2.284 -0.042

CO2 5.472e-004 5.484e-004 -3.262 -3.261 0.001

CaHCO3+ 7.484e-005 6.797e-005 -4.126 -4.168 -0.042

MgHCO3+ 4.453e-005 4.031e-005 -4.351 -4.395 -0.043

CaCO3 8.634e-006 8.653e-006 -5.064 -5.063 0.001

CO3-2 6.999e-006 4.761e-006 -5.155 -5.322 -0.167

MgCO3 2.592e-006 2.598e-006 -5.586 -5.585 0.001

NaHCO3 6.744e-007 6.759e-007 -6.171 -6.170 0.001

SrHCO3+ 6.442e-007 5.850e-007 -6.191 -6.233 -0.042

SrCO3 2.358e-008 2.364e-008 -7.627 -7.626 0.001

NaCO3- 1.204e-008 1.090e-008 -7.919 -7.963 -0.043

BaHCO3+ 9.131e-009 8.266e-009 -8.039 -8.083 -0.043

BaCO3 4.663e-010 4.674e-010 -9.331 -9.330 0.001

Ca 2.044e-003

Ca+2 1.910e-003 1.298e-003 -2.719 -2.887 -0.168

CaHCO3+ 7.484e-005 6.797e-005 -4.126 -4.168 -0.042

CaSO4 5.099e-005 5.110e-005 -4.293 -4.292 0.001

CaCO3 8.634e-006 8.653e-006 -5.064 -5.063 0.001

CaOH+ 6.158e-009 5.574e-009 -8.211 -8.254 -0.043

CaHSO4+ 1.121e-011 1.015e-011 -10.950 -10.994 -0.043

Cl 8.805e-005

Cl- 8.805e-005 7.957e-005 -4.055 -4.099 -0.044

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.323 -43.322 0.001

K 2.984e-005

K+ 2.980e-005 2.693e-005 -4.526 -4.570 -0.044

KSO4- 3.725e-008 3.372e-008 -7.429 -7.472 -0.043

KOH 2.410e-012 2.415e-012 -11.618 -11.617 0.001

Li 4.614e-006

Li+ 4.610e-006 4.193e-006 -5.336 -5.378 -0.041

LiSO4- 4.482e-009 4.057e-009 -8.349 -8.392 -0.043

LiOH 2.479e-012 2.485e-012 -11.606 -11.605 0.001

Mg 1.078e-003

Mg+2 1.005e-003 6.876e-004 -2.998 -3.163 -0.165

MgHCO3+ 4.453e-005 4.031e-005 -4.351 -4.395 -0.043

MgSO4 2.584e-005 2.589e-005 -4.588 -4.587 0.001

MgCO3 2.592e-006 2.598e-006 -5.586 -5.585 0.001

MgOH+ 2.307e-008 2.088e-008 -7.637 -7.680 -0.043

N(5) 1.929e-006

NO3- 1.929e-006 1.740e-006 -5.715 -5.760 -0.045

Na 2.559e-004

Na+ 2.550e-004 2.310e-004 -3.594 -3.636 -0.043

NaHCO3 6.744e-007 6.759e-007 -6.171 -6.170 0.001

NaSO4- 2.620e-007 2.371e-007 -6.582 -6.625 -0.043

NaCO3- 1.204e-008 1.090e-008 -7.919 -7.963 -0.043

NaOH 3.940e-011 3.949e-011 -10.405 -10.404 0.001

O(0) 3.373e-010

O2 1.687e-010 1.690e-010 -9.773 -9.772 0.001

S(6) 4.052e-004

SO4-2 3.276e-004 2.217e-004 -3.485 -3.654 -0.170

CaSO4 5.099e-005 5.110e-005 -4.293 -4.292 0.001

MgSO4 2.584e-005 2.589e-005 -4.588 -4.587 0.001

SrSO4 4.126e-007 4.136e-007 -6.384 -6.383 0.001

NaSO4- 2.620e-007 2.371e-007 -6.582 -6.625 -0.043

KSO4- 3.725e-008 3.372e-008 -7.429 -7.472 -0.043

BaSO4 2.681e-008 2.687e-008 -7.572 -7.571 0.001

LiSO4- 4.482e-009 4.057e-009 -8.349 -8.392 -0.043

HSO4- 7.179e-010 6.499e-010 -9.144 -9.187 -0.043

CaHSO4+ 1.121e-011 1.015e-011 -10.950 -10.994 -0.043

Si 9.475e-005

H4SiO4 9.450e-005 9.471e-005 -4.025 -4.024 0.001

H3SiO4- 2.540e-007 2.299e-007 -6.595 -6.638 -0.043

H2SiO4-2 2.602e-013 1.747e-013 -12.585 -12.758 -0.173

Sr 1.736e-005

Sr+2 1.628e-005 1.109e-005 -4.788 -4.955 -0.167

SrHCO3+ 6.442e-007 5.850e-007 -6.191 -6.233 -0.042

SrSO4 4.126e-007 4.136e-007 -6.384 -6.383 0.001

SrCO3 2.358e-008 2.364e-008 -7.627 -7.626 0.001

SrOH+ 1.621e-011 1.471e-011 -10.790 -10.832 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.21 -6.54 -4.33 CaSO4

Aragonite 0.06 -8.21 -8.27 CaCO3

Barite -0.09 -10.27 -10.18 BaSO4

Calcite 0.21 -8.21 -8.42 CaCO3

Celestite -1.99 -8.61 -6.62 SrSO4

Chalcedony -0.33 -4.02 -3.70 SiO2

Chrysotile -6.81 26.94 33.75 Mg3Si2O5(OH)4

CO2(g) -1.95 -3.26 -1.31 CO2

Dolomite 0.11 -16.69 -16.80 CaMg(CO3)2

Gypsum -1.95 -6.54 -4.59 CaSO4:2H2O

H2(g) -40.23 -43.32 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.29 -7.74 1.55 NaCl

O2(g) -6.98 -9.77 -2.79 O2

Quartz 0.14 -4.02 -4.16 SiO2

Sepiolite -4.83 11.26 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -7.40 11.26 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.21 -4.02 -2.81 SiO2

Strontianite -1.00 -10.28 -9.28 SrCO3

Talc -3.93 18.89 22.82 Mg3Si4O10(OH)2

Witherite -3.33 -11.94 -8.61 BaCO3

Initial solution 8. 07-9-22

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 3.449e-006 3.449e-006

Alkalinity 6.133e-003 6.133e-003

B 5.183e-006 5.183e-006

Ba 8.669e-007 8.669e-007

Ca 2.389e-003 2.389e-003

Cl 6.801e-005 6.801e-005

K 2.574e-005 2.574e-005

Li 4.326e-006 4.326e-006

Mg 8.107e-004 8.107e-004

N(5) 3.214e-006 3.214e-006

Na 2.006e-004 2.006e-004

S(6) 3.718e-004 3.718e-004

Si 9.891e-005 9.891e-005

Sr 9.706e-006 9.706e-006

----------------------------Description of solution----------------------------

pH = 7.275 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 450

Density (g/cm3) = 0.99983

Activity of water = 1.000

Ionic strength = 9.812e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.885e-003

Total CO2 (mol/kg) = 6.885e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -2.857e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.20

Iterations = 10

Total H = 1.110189e+002

Total O = 5.552801e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 7.942e-008 7.169e-008 -7.100 -7.145 -0.044

H+ 5.792e-008 5.303e-008 -7.237 -7.275 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 3.449e-006

Al(OH)4- 3.256e-006 2.945e-006 -5.487 -5.531 -0.044

Al(OH)2+ 9.703e-008 8.777e-008 -7.013 -7.057 -0.044

Al(OH)3 9.324e-008 9.345e-008 -7.030 -7.029 0.001

AlOH+2 2.736e-009 1.832e-009 -8.563 -8.737 -0.174

Al+3 4.824e-011 2.180e-011 -10.317 -10.662 -0.345

AlSO4+ 1.309e-011 1.184e-011 -10.883 -10.927 -0.044

Al(SO4)2- 7.892e-014 7.139e-014 -13.103 -13.146 -0.044

AlHSO4+2 7.630e-020 5.108e-020 -19.117 -19.292 -0.174

B 5.183e-006

H3BO3 5.134e-006 5.146e-006 -5.290 -5.289 0.001

H2BO3- 4.913e-008 4.444e-008 -7.309 -7.352 -0.044

Ba 8.669e-007

Ba+2 7.912e-007 5.344e-007 -6.102 -6.272 -0.170

BaSO4 5.399e-008 5.411e-008 -7.268 -7.267 0.001

BaHCO3+ 2.100e-008 1.900e-008 -7.678 -7.721 -0.044

BaCO3 7.813e-010 7.830e-010 -9.107 -9.106 0.001

BaOH+ 3.774e-013 3.414e-013 -12.423 -12.467 -0.044

C(4) 6.885e-003

HCO3- 5.963e-003 5.412e-003 -2.225 -2.267 -0.042

CO2 7.809e-004 7.827e-004 -3.107 -3.106 0.001

CaHCO3+ 9.095e-005 8.254e-005 -4.041 -4.083 -0.042

MgHCO3+ 3.480e-005 3.148e-005 -4.458 -4.502 -0.044

CaCO3 7.642e-006 7.659e-006 -5.117 -5.116 0.001

CO3-2 5.321e-006 3.609e-006 -5.274 -5.443 -0.169

MgCO3 1.475e-006 1.479e-006 -5.831 -5.830 0.001

NaHCO3 5.496e-007 5.508e-007 -6.260 -6.259 0.001

SrHCO3+ 3.743e-007 3.397e-007 -6.427 -6.469 -0.042

BaHCO3+ 2.100e-008 1.900e-008 -7.678 -7.721 -0.044

SrCO3 9.982e-009 1.000e-008 -8.001 -8.000 0.001

NaCO3- 7.158e-009 6.475e-009 -8.145 -8.189 -0.044

BaCO3 7.813e-010 7.830e-010 -9.107 -9.106 0.001

Ca 2.389e-003

Ca+2 2.236e-003 1.516e-003 -2.650 -2.819 -0.169

CaHCO3+ 9.095e-005 8.254e-005 -4.041 -4.083 -0.042

CaSO4 5.425e-005 5.438e-005 -4.266 -4.265 0.001

CaCO3 7.642e-006 7.659e-006 -5.117 -5.116 0.001

CaOH+ 5.244e-009 4.743e-009 -8.280 -8.324 -0.044

CaHSO4+ 1.637e-011 1.481e-011 -10.786 -10.829 -0.044

Cl 6.801e-005

Cl- 6.801e-005 6.142e-005 -4.167 -4.212 -0.044

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.048 -43.047 0.001

K 2.574e-005

K+ 2.571e-005 2.322e-005 -4.590 -4.634 -0.044

KSO4- 2.930e-008 2.650e-008 -7.533 -7.577 -0.044

KOH 1.514e-012 1.518e-012 -11.820 -11.819 0.001

Li 4.326e-006

Li+ 4.322e-006 3.928e-006 -5.364 -5.406 -0.041

LiSO4- 3.830e-009 3.465e-009 -8.417 -8.460 -0.044

LiOH 1.693e-012 1.697e-012 -11.771 -11.770 0.001

Mg 8.107e-004

Mg+2 7.568e-004 5.162e-004 -3.121 -3.287 -0.166

MgHCO3+ 3.480e-005 3.148e-005 -4.458 -4.502 -0.044

MgSO4 1.768e-005 1.772e-005 -4.753 -4.752 0.001

MgCO3 1.475e-006 1.479e-006 -5.831 -5.830 0.001

MgOH+ 1.263e-008 1.143e-008 -7.899 -7.942 -0.044

N(5) 3.214e-006

NO3- 3.214e-006 2.897e-006 -5.493 -5.538 -0.045

Na 2.006e-004

Na+ 1.999e-004 1.810e-004 -3.699 -3.742 -0.043

NaHCO3 5.496e-007 5.508e-007 -6.260 -6.259 0.001

NaSO4- 1.872e-007 1.693e-007 -6.728 -6.771 -0.044

NaCO3- 7.158e-009 6.475e-009 -8.145 -8.189 -0.044

NaOH 2.250e-011 2.255e-011 -10.648 -10.647 0.001

O(0) 9.519e-011

O2 4.759e-011 4.770e-011 -10.322 -10.321 0.001

S(6) 3.718e-004

SO4-2 2.994e-004 2.020e-004 -3.524 -3.695 -0.171

CaSO4 5.425e-005 5.438e-005 -4.266 -4.265 0.001

MgSO4 1.768e-005 1.772e-005 -4.753 -4.752 0.001

SrSO4 2.100e-007 2.104e-007 -6.678 -6.677 0.001

NaSO4- 1.872e-007 1.693e-007 -6.728 -6.771 -0.044

BaSO4 5.399e-008 5.411e-008 -7.268 -7.267 0.001

KSO4- 2.930e-008 2.650e-008 -7.533 -7.577 -0.044

LiSO4- 3.830e-009 3.465e-009 -8.417 -8.460 -0.044

HSO4- 8.984e-010 8.126e-010 -9.047 -9.090 -0.044

CaHSO4+ 1.637e-011 1.481e-011 -10.786 -10.829 -0.044

AlSO4+ 1.309e-011 1.184e-011 -10.883 -10.927 -0.044

Al(SO4)2- 7.892e-014 7.139e-014 -13.103 -13.146 -0.044

AlHSO4+2 7.630e-020 5.108e-020 -19.117 -19.292 -0.174

Si 9.891e-005

H4SiO4 9.872e-005 9.894e-005 -4.006 -4.005 0.001

H3SiO4- 1.935e-007 1.751e-007 -6.713 -6.757 -0.044

H2SiO4-2 1.449e-013 9.699e-014 -12.839 -13.013 -0.174

Sr 9.706e-006

Sr+2 9.112e-006 6.189e-006 -5.040 -5.208 -0.168

SrHCO3+ 3.743e-007 3.397e-007 -6.427 -6.469 -0.042

SrSO4 2.100e-007 2.104e-007 -6.678 -6.677 0.001

SrCO3 9.982e-009 1.000e-008 -8.001 -8.000 0.001

SrOH+ 6.601e-012 5.984e-012 -11.180 -11.223 -0.043

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -0.45 11.16 11.61 Al(OH)3

Albite -2.49 -21.29 -18.80 NaAlSi3O8

Alunite -0.50 -0.36 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.18 -6.51 -4.33 CaSO4

Anorthite -1.82 -21.89 -20.07 CaAl2Si2O8

Aragonite 0.01 -8.26 -8.27 CaCO3

Barite 0.22 -9.97 -10.18 BaSO4

Ca-Montmorillonite 4.22 -42.60 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.16 -8.26 -8.42 CaCO3

Celestite -2.28 -8.90 -6.62 SrSO4

Chalcedony -0.31 -4.00 -3.70 SiO2

Chlorite(14A) -6.40 66.63 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -7.97 25.78 33.75 Mg3Si2O5(OH)4

CO2(g) -1.79 -3.11 -1.31 CO2

Dolomite -0.19 -16.99 -16.80 CaMg(CO3)2

Gibbsite 2.35 11.16 8.81 Al(OH)3

Gypsum -1.93 -6.51 -4.59 CaSO4:2H2O

H2(g) -39.95 -43.05 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.51 -7.95 1.55 NaCl

Illite 2.88 -39.07 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -0.66 -22.18 -21.52 KAlSi3O8

K-mica 9.59 24.12 14.53 KAl3Si3O10(OH)2

Kaolinite 5.80 14.32 8.52 Al2Si2O5(OH)4

O2(g) -7.53 -10.32 -2.79 O2

Quartz 0.16 -4.00 -4.16 SiO2

Sepiolite -5.58 10.51 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.15 10.51 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.19 -4.00 -2.81 SiO2

Strontianite -1.37 -10.65 -9.28 SrCO3

Talc -5.05 17.77 22.82 Mg3Si4O10(OH)2

Witherite -3.10 -11.71 -8.61 BaCO3

Initial solution 9. 07-10-28

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 1.483e-007 1.483e-007

Alkalinity 6.133e-003 6.133e-003

B 3.425e-006 3.425e-006

Ba 9.107e-007 9.107e-007

Ca 2.574e-003 2.574e-003

Cl 7.564e-005 7.564e-005

K 2.405e-005 2.405e-005

Li 4.182e-006 4.182e-006

Mg 8.190e-004 8.190e-004

N(5) 2.214e-006 2.214e-006

Na 2.106e-004 2.106e-004

S(6) 4.645e-004 4.645e-004

Si 1.042e-004 1.042e-004

Sr 1.085e-005 1.085e-005

----------------------------Description of solution----------------------------

pH = 7.272 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 469

Density (g/cm3) = 0.99985

Activity of water = 1.000

Ionic strength = 1.030e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.903e-003

Total CO2 (mol/kg) = 6.903e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -9.117e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.67

Iterations = 10

Total H = 1.110190e+002

Total O = 5.552843e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 7.898e-008 7.113e-008 -7.102 -7.148 -0.045

H+ 5.848e-008 5.345e-008 -7.233 -7.272 -0.039

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 1.483e-007

Al(OH)4- 1.399e-007 1.263e-007 -6.854 -6.899 -0.045

Al(OH)2+ 4.236e-009 3.824e-009 -8.373 -8.418 -0.045

Al(OH)3 4.030e-009 4.040e-009 -8.395 -8.394 0.001

AlOH+2 1.212e-010 8.044e-011 -9.917 -10.095 -0.178

Al+3 2.167e-012 9.645e-013 -11.664 -12.016 -0.352

AlSO4+ 7.139e-013 6.444e-013 -12.146 -12.191 -0.045

Al(SO4)2- 5.292e-015 4.777e-015 -14.276 -14.321 -0.045

AlHSO4+2 4.221e-021 2.801e-021 -20.375 -20.553 -0.178

B 3.425e-006

H3BO3 3.392e-006 3.400e-006 -5.469 -5.468 0.001

H2BO3- 3.229e-008 2.914e-008 -7.491 -7.535 -0.045

Ba 9.107e-007

Ba+2 8.200e-007 5.493e-007 -6.086 -6.260 -0.174

BaSO4 6.823e-008 6.839e-008 -7.166 -7.165 0.001

BaHCO3+ 2.162e-008 1.951e-008 -7.665 -7.710 -0.045

BaCO3 7.960e-010 7.978e-010 -9.099 -9.098 0.001

BaOH+ 3.857e-013 3.482e-013 -12.414 -12.458 -0.045

C(4) 6.903e-003

HCO3- 5.969e-003 5.406e-003 -2.224 -2.267 -0.043

CO2 7.862e-004 7.881e-004 -3.104 -3.103 0.001

CaHCO3+ 9.685e-005 8.771e-005 -4.014 -4.057 -0.043

MgHCO3+ 3.476e-005 3.138e-005 -4.459 -4.503 -0.045

CaCO3 8.057e-006 8.076e-006 -5.094 -5.093 0.001

CO3-2 5.317e-006 3.578e-006 -5.274 -5.446 -0.172

MgCO3 1.459e-006 1.463e-006 -5.836 -5.835 0.001

NaHCO3 5.751e-007 5.764e-007 -6.240 -6.239 0.001

SrHCO3+ 4.136e-007 3.746e-007 -6.383 -6.426 -0.043

BaHCO3+ 2.162e-008 1.951e-008 -7.665 -7.710 -0.045

SrCO3 1.092e-008 1.095e-008 -7.962 -7.961 0.001

NaCO3- 7.449e-009 6.723e-009 -8.128 -8.172 -0.045

BaCO3 7.960e-010 7.978e-010 -9.099 -9.098 0.001

Ca 2.574e-003

Ca+2 2.398e-003 1.612e-003 -2.620 -2.793 -0.172

CaHCO3+ 9.685e-005 8.771e-005 -4.014 -4.057 -0.043

CaSO4 7.095e-005 7.112e-005 -4.149 -4.148 0.001

CaCO3 8.057e-006 8.076e-006 -5.094 -5.093 0.001

CaOH+ 5.546e-009 5.006e-009 -8.256 -8.300 -0.045

CaHSO4+ 2.163e-011 1.952e-011 -10.665 -10.709 -0.045

Cl 7.564e-005

Cl- 7.564e-005 6.814e-005 -4.121 -4.167 -0.045

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.041 -43.040 0.001

K 2.405e-005

K+ 2.402e-005 2.164e-005 -4.619 -4.665 -0.045

KSO4- 3.365e-008 3.037e-008 -7.473 -7.518 -0.045

KOH 1.400e-012 1.404e-012 -11.854 -11.853 0.001

Li 4.182e-006

Li+ 4.177e-006 3.789e-006 -5.379 -5.421 -0.042

LiSO4- 4.553e-009 4.110e-009 -8.342 -8.386 -0.045

LiOH 1.620e-012 1.624e-012 -11.790 -11.789 0.001

Mg 8.190e-004

Mg+2 7.611e-004 5.151e-004 -3.119 -3.288 -0.170

MgHCO3+ 3.476e-005 3.138e-005 -4.459 -4.503 -0.045

MgSO4 2.169e-005 2.174e-005 -4.664 -4.663 0.001

MgCO3 1.459e-006 1.463e-006 -5.836 -5.835 0.001

MgOH+ 1.253e-008 1.131e-008 -7.902 -7.946 -0.045

N(5) 2.214e-006

NO3- 2.214e-006 1.991e-006 -5.655 -5.701 -0.046

Na 2.106e-004

Na+ 2.098e-004 1.896e-004 -3.678 -3.722 -0.044

NaHCO3 5.751e-007 5.764e-007 -6.240 -6.239 0.001

NaSO4- 2.416e-007 2.181e-007 -6.617 -6.661 -0.045

NaCO3- 7.449e-009 6.723e-009 -8.128 -8.172 -0.045

NaOH 2.338e-011 2.343e-011 -10.631 -10.630 0.001

O(0) 9.225e-011

O2 4.613e-011 4.623e-011 -10.336 -10.335 0.001

S(6) 4.645e-004

SO4-2 3.713e-004 2.484e-004 -3.430 -3.605 -0.174

CaSO4 7.095e-005 7.112e-005 -4.149 -4.148 0.001

MgSO4 2.169e-005 2.174e-005 -4.664 -4.663 0.001

SrSO4 2.849e-007 2.856e-007 -6.545 -6.544 0.001

NaSO4- 2.416e-007 2.181e-007 -6.617 -6.661 -0.045

BaSO4 6.823e-008 6.839e-008 -7.166 -7.165 0.001

KSO4- 3.365e-008 3.037e-008 -7.473 -7.518 -0.045

LiSO4- 4.553e-009 4.110e-009 -8.342 -8.386 -0.045

HSO4- 1.116e-009 1.007e-009 -8.952 -8.997 -0.045

CaHSO4+ 2.163e-011 1.952e-011 -10.665 -10.709 -0.045

AlSO4+ 7.139e-013 6.444e-013 -12.146 -12.191 -0.045

Al(SO4)2- 5.292e-015 4.777e-015 -14.276 -14.321 -0.045

AlHSO4+2 4.221e-021 2.801e-021 -20.375 -20.553 -0.178

Si 1.042e-004

H4SiO4 1.040e-004 1.043e-004 -3.983 -3.982 0.001

H3SiO4- 2.028e-007 1.831e-007 -6.693 -6.737 -0.045

H2SiO4-2 1.516e-013 1.006e-013 -12.819 -12.997 -0.178

Sr 1.085e-005

Sr+2 1.014e-005 6.831e-006 -4.994 -5.166 -0.172

SrHCO3+ 4.136e-007 3.746e-007 -6.383 -6.426 -0.043

SrSO4 2.849e-007 2.856e-007 -6.545 -6.544 0.001

SrCO3 1.092e-008 1.095e-008 -7.962 -7.961 0.001

SrOH+ 7.244e-012 6.554e-012 -11.140 -11.184 -0.044

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -1.81 9.80 11.61 Al(OH)3

Albite -3.77 -22.57 -18.80 NaAlSi3O8

Alunite -4.43 -4.29 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.06 -6.40 -4.33 CaSO4

Anorthite -4.48 -24.55 -20.07 CaAl2Si2O8

Aragonite 0.03 -8.24 -8.27 CaCO3

Barite 0.32 -9.86 -10.18 BaSO4

Ca-Montmorillonite 1.13 -45.69 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.18 -8.24 -8.42 CaCO3

Celestite -2.15 -8.77 -6.62 SrSO4

Chalcedony -0.29 -3.98 -3.70 SiO2

Chlorite(14A) -9.10 63.94 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -7.94 25.80 33.75 Mg3Si2O5(OH)4

CO2(g) -1.79 -3.10 -1.31 CO2

Dolomite -0.17 -16.97 -16.80 CaMg(CO3)2

Gibbsite 0.99 9.80 8.81 Al(OH)3

Gypsum -1.81 -6.40 -4.59 CaSO4:2H2O

H2(g) -39.94 -43.04 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.44 -7.89 1.55 NaCl

Illite -0.20 -42.15 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -1.99 -23.51 -21.52 KAlSi3O8

K-mica 5.54 20.06 14.53 KAl3Si3O10(OH)2

Kaolinite 3.12 11.64 8.52 Al2Si2O5(OH)4

O2(g) -7.54 -10.34 -2.79 O2

Quartz 0.18 -3.98 -4.16 SiO2

Sepiolite -5.52 10.57 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.09 10.57 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.17 -3.98 -2.81 SiO2

Strontianite -1.33 -10.61 -9.28 SrCO3

Talc -4.98 17.84 22.82 Mg3Si4O10(OH)2

Witherite -3.10 -11.71 -8.61 BaCO3

Initial solution 10. 07-11-18

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 7.046e-007 7.046e-007

Alkalinity 6.395e-003 6.395e-003

B 3.425e-006 3.425e-006

Ba 8.888e-007 8.888e-007

Ca 2.704e-003 2.704e-003

Cl 6.773e-005 6.773e-005

K 2.364e-005 2.364e-005

Li 4.182e-006 4.182e-006

Mg 8.972e-004 8.972e-004

Na 2.176e-004 2.176e-004

S(6) 4.708e-004 4.708e-004

Si 1.004e-004 1.004e-004

Sr 1.108e-005 1.108e-005

----------------------------Description of solution----------------------------

pH = 7.314 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 489

Density (g/cm3) = 0.99987

Activity of water = 1.000

Ionic strength = 1.081e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.115e-003

Total CO2 (mol/kg) = 7.115e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = 6.874e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.49

Iterations = 11

Total H = 1.110192e+002

Total O = 5.552912e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.727e-008 7.842e-008 -7.059 -7.106 -0.046

H+ 5.313e-008 4.848e-008 -7.275 -7.314 -0.040

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 7.046e-007

Al(OH)4- 6.700e-007 6.034e-007 -6.174 -6.219 -0.045

Al(OH)3 1.746e-008 1.751e-008 -7.758 -7.757 0.001

Al(OH)2+ 1.669e-008 1.503e-008 -7.778 -7.823 -0.045

AlOH+2 4.359e-010 2.868e-010 -9.361 -9.542 -0.182

Al+3 7.116e-012 3.119e-012 -11.148 -11.506 -0.358

AlSO4+ 2.306e-012 2.077e-012 -11.637 -11.683 -0.045

Al(SO4)2- 1.704e-014 1.534e-014 -13.769 -13.814 -0.045

AlHSO4+2 1.245e-020 8.190e-021 -19.905 -20.087 -0.182

B 3.425e-006

H3BO3 3.389e-006 3.398e-006 -5.470 -5.469 0.001

H2BO3- 3.564e-008 3.210e-008 -7.448 -7.493 -0.045

Ba 8.888e-007

Ba+2 8.004e-007 5.316e-007 -6.097 -6.274 -0.178

BaSO4 6.581e-008 6.597e-008 -7.182 -7.181 0.001

BaHCO3+ 2.177e-008 1.961e-008 -7.662 -7.708 -0.045

BaCO3 8.819e-010 8.841e-010 -9.055 -9.054 0.001

BaOH+ 4.125e-013 3.715e-013 -12.385 -12.430 -0.045

C(4) 7.115e-003

HCO3- 6.212e-003 5.614e-003 -2.207 -2.251 -0.044

CO2 7.405e-004 7.423e-004 -3.130 -3.129 0.001

CaHCO3+ 1.049e-004 9.478e-005 -3.979 -4.023 -0.044

MgHCO3+ 3.927e-005 3.537e-005 -4.406 -4.451 -0.045

CaCO3 9.596e-006 9.620e-006 -5.018 -5.017 0.001

CO3-2 6.138e-006 4.096e-006 -5.212 -5.388 -0.176

MgCO3 1.813e-006 1.817e-006 -5.742 -5.741 0.001

NaHCO3 6.155e-007 6.170e-007 -6.211 -6.210 0.001

SrHCO3+ 4.355e-007 3.936e-007 -6.361 -6.405 -0.044

BaHCO3+ 2.177e-008 1.961e-008 -7.662 -7.708 -0.045

SrCO3 1.265e-008 1.268e-008 -7.898 -7.897 0.001

NaCO3- 8.809e-009 7.934e-009 -8.055 -8.101 -0.045

BaCO3 8.819e-010 8.841e-010 -9.055 -9.054 0.001

Ca 2.704e-003

Ca+2 2.516e-003 1.678e-003 -2.599 -2.775 -0.176

CaHCO3+ 1.049e-004 9.478e-005 -3.979 -4.023 -0.044

CaSO4 7.357e-005 7.375e-005 -4.133 -4.132 0.001

CaCO3 9.596e-006 9.620e-006 -5.018 -5.017 0.001

CaOH+ 6.376e-009 5.743e-009 -8.195 -8.241 -0.045

CaHSO4+ 2.039e-011 1.836e-011 -10.691 -10.736 -0.045

Cl 6.773e-005

Cl- 6.773e-005 6.089e-005 -4.169 -4.215 -0.046

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.126 -43.125 0.001

K 2.364e-005

K+ 2.361e-005 2.122e-005 -4.627 -4.673 -0.046

KSO4- 3.296e-008 2.969e-008 -7.482 -7.527 -0.045

KOH 1.514e-012 1.518e-012 -11.820 -11.819 0.001

Li 4.182e-006

Li+ 4.177e-006 3.782e-006 -5.379 -5.422 -0.043

LiSO4- 4.538e-009 4.088e-009 -8.343 -8.389 -0.045

LiOH 1.782e-012 1.787e-012 -11.749 -11.748 0.001

Mg 8.972e-004

Mg+2 8.326e-004 5.591e-004 -3.080 -3.253 -0.173

MgHCO3+ 3.927e-005 3.537e-005 -4.406 -4.451 -0.045

MgSO4 2.346e-005 2.352e-005 -4.630 -4.629 0.001

MgCO3 1.813e-006 1.817e-006 -5.742 -5.741 0.001

MgOH+ 1.503e-008 1.354e-008 -7.823 -7.868 -0.045

Na 2.176e-004

Na+ 2.167e-004 1.954e-004 -3.664 -3.709 -0.045

NaHCO3 6.155e-007 6.170e-007 -6.211 -6.210 0.001

NaSO4- 2.488e-007 2.240e-007 -6.604 -6.650 -0.045

NaCO3- 8.809e-009 7.934e-009 -8.055 -8.101 -0.045

NaOH 2.656e-011 2.663e-011 -10.576 -10.575 0.001

O(0) 1.362e-010

O2 6.812e-011 6.829e-011 -10.167 -10.166 0.001

S(6) 4.708e-004

SO4-2 3.731e-004 2.476e-004 -3.428 -3.606 -0.178

CaSO4 7.357e-005 7.375e-005 -4.133 -4.132 0.001

MgSO4 2.346e-005 2.352e-005 -4.630 -4.629 0.001

SrSO4 2.873e-007 2.880e-007 -6.542 -6.541 0.001

NaSO4- 2.488e-007 2.240e-007 -6.604 -6.650 -0.045

BaSO4 6.581e-008 6.597e-008 -7.182 -7.181 0.001

KSO4- 3.296e-008 2.969e-008 -7.482 -7.527 -0.045

LiSO4- 4.538e-009 4.088e-009 -8.343 -8.389 -0.045

HSO4- 1.011e-009 9.104e-010 -8.995 -9.041 -0.045

CaHSO4+ 2.039e-011 1.836e-011 -10.691 -10.736 -0.045

AlSO4+ 2.306e-012 2.077e-012 -11.637 -11.683 -0.045

Al(SO4)2- 1.704e-014 1.534e-014 -13.769 -13.814 -0.045

AlHSO4+2 1.245e-020 8.190e-021 -19.905 -20.087 -0.182

Si 1.004e-004

H4SiO4 1.002e-004 1.005e-004 -3.999 -3.998 0.001

H3SiO4- 2.159e-007 1.944e-007 -6.666 -6.711 -0.045

H2SiO4-2 1.791e-013 1.178e-013 -12.747 -12.929 -0.182

Sr 1.108e-005

Sr+2 1.034e-005 6.911e-006 -4.985 -5.160 -0.175

SrHCO3+ 4.355e-007 3.936e-007 -6.361 -6.405 -0.044

SrSO4 2.873e-007 2.880e-007 -6.542 -6.541 0.001

SrCO3 1.265e-008 1.268e-008 -7.898 -7.897 0.001

SrOH+ 8.097e-012 7.310e-012 -11.092 -11.136 -0.044

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -1.18 10.44 11.61 Al(OH)3

Albite -3.12 -21.92 -18.80 NaAlSi3O8

Alunite -2.66 -2.52 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.05 -6.38 -4.33 CaSO4

Anorthite -3.14 -23.21 -20.07 CaAl2Si2O8

Aragonite 0.11 -8.16 -8.27 CaCO3

Barite 0.30 -9.88 -10.18 BaSO4

Ca-Montmorillonite 2.57 -44.25 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.26 -8.16 -8.42 CaCO3

Celestite -2.14 -8.77 -6.62 SrSO4

Chalcedony -0.30 -4.00 -3.70 SiO2

Chlorite(14A) -7.27 65.76 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -7.62 26.13 33.75 Mg3Si2O5(OH)4

CO2(g) -1.82 -3.13 -1.31 CO2

Dolomite -0.00 -16.80 -16.80 CaMg(CO3)2

Gibbsite 1.63 10.44 8.81 Al(OH)3

Gypsum -1.79 -6.38 -4.59 CaSO4:2H2O

H2(g) -40.03 -43.12 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.48 -7.92 1.55 NaCl

Illite 1.26 -40.69 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -1.37 -22.89 -21.52 KAlSi3O8

K-mica 7.43 21.96 14.53 KAl3Si3O10(OH)2

Kaolinite 4.36 12.88 8.52 Al2Si2O5(OH)4

O2(g) -7.37 -10.17 -2.79 O2

Quartz 0.17 -4.00 -4.16 SiO2

Sepiolite -5.33 10.76 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -7.90 10.76 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.18 -4.00 -2.81 SiO2

Strontianite -1.27 -10.55 -9.28 SrCO3

Talc -4.69 18.14 22.82 Mg3Si4O10(OH)2

Witherite -3.05 -11.66 -8.61 BaCO3

------------------

End of simulation.

------------------

------------------------------------

Reading input data for simulation 2.

------------------------------------

-----------

End of run.

Input file: C:\Users\huan\Desktop\Phreeqc calculation Konza\3-5 Well\2008-09 3-5\2008-09 3-5.pqi

Output file: C:\Users\huan\Desktop\Phreeqc calculation Konza\3-5 Well\2008-09 3-5\2008-09 3-5.pqo

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

------------------

Reading data base.

------------------

SOLUTION\_MASTER\_SPECIES

SOLUTION\_SPECIES

PHASES

EXCHANGE\_MASTER\_SPECIES

EXCHANGE\_SPECIES

SURFACE\_MASTER\_SPECIES

SURFACE\_SPECIES

RATES

END

------------------------------------

Reading input data for simulation 1.

------------------------------------

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

SOLUTION 1 08-4-6

temp 13

pH 7 Calcite 0.777

pe 12.7

redox pe

units ppm

density 1

Ca 87.7

K 0.833

Mg 18.6

Na 4.25

Al 0.002

Sr 0.78

B 0.02

Ba 0.09

Li 0.026

Si 4.63

S(6) 21

Cl 2.29

Alkalinity 349 as HCO3

water 1 # kg

SOLUTION 2 08-5-20

temp 13

pH 7 Calcite 0.623

pe 12.7

redox pe

units ppm

density 1

Ca 92.4

K 0.883

Mg 19.4

Na 4.3

Al 0.386

Sr 0.81

B 0.024

Ba 0.1

Li 0.03

Si 5.98

S(6) 20.7

Cl 2.54

Alkalinity 363 as HCO3

water 1 # kg

SOLUTION 3 08-6-21

temp 13

pH 7 Calcite 0.476

pe 12.7

redox pe

units ppm

density 1

Ca 95.1

K 0.887

Mg 19.8

Na 4.76

Sr 0.84

B 0.029

Ba 0.106

Li 0.032

Si 5.79

N(5) 0.043

S(6) 15.5

Cl 2.52

Alkalinity 389 as HCO3

water 1 # kg

SOLUTION 4 08-8-7

temp 13

pH 7 Calcite 0.271

pe 12.7

redox pe

units ppm

density 1

Ca 95.1

K 0.947

Mg 19.4

Na 4.38

Al 0.006

Sr 0.86

B 0.035

Ba 0.112

Li 0.034

Si 6.27

N(5) 0.048

S(6) 16.4

Cl 2.38

Alkalinity 392 as HCO3

water 1 # kg

SOLUTION 5 08-9-21

temp 13

pH 7 Calcite 0.16

pe 12.7

redox pe

units ppm

density 1

Ca 90.7

K 0.954

Mg 18.3

Na 4.45

Sr 0.84

B 0.032

Ba 0.117

Li 0.046

Si 6.07

N(5) 0.048

S(6) 15.1

Cl 2.21

Alkalinity 375 as HCO3

water 1 # kg

SOLUTION 6 08-11-2

temp 13

pH 7 Calcite 0.2

pe 12.7

redox pe

units ppm

density 1

Ca 92.3

K 0.912

Mg 19.2

Na 4.5

Al 0.127

Sr 0.87

B 0.026

Ba 0.112

Li 0.029

Si 6.2

N(5) 0.031

S(6) 20.4

Cl 1.5

Alkalinity 376 as HCO3

water 1 # kg

SOLUTION 7 08-11-30

temp 13

pH 7 Calcite 0.334

pe 12.7

redox pe

units ppm

density 1

Ca 92.4

K 0.859

Mg 18.5

Na 4.24

Al 0.2

Sr 0.84

B 0.024

Ba 0.106

Li 0.042

Si 5.9

N(5) 0.068

S(6) 21.9

Cl 2.59

Alkalinity 365 as HCO3

water 1 # kg

SOLUTION 8 09-1-6

temp 13

pH 7 Calcite 0.635

pe 12.7

redox pe

units ppm

density 1

Ca 88.8

K 0.357

Mg 18.2

Na 4.26

Al 0.222

Sr 0.81

B 0.017

Ba 0.098

Li 0.01

Si 5.16

N(5) 0.031

S(6) 26.8

Cl 2.16

Alkalinity 357 as HCO3

water 1 # kg

SOLUTION 9 09-2-21

temp 13

pH 7 Calcite 0.811

pe 12.7

redox pe

units ppm

density 1

Ca 92.3

K 0.424

Mg 18.7

Na 4.26

Al 0.128

Sr 0.82

B 0.016

Ba 0.095

Li 0.037

Si 4.88

N(5) 0.062

S(6) 33.4

Cl 2.25

Alkalinity 353 as HCO3

water 1 # kg

SOLUTION 10 09-4-18

temp 13

pH 7 Calcite 0.747

pe 12.7

redox pe

units ppm

density 1

Ca 90.9

K 0.477

Mg 18.3

Na 4.36

Al 0.458

Sr 0.78

B 0.019

Ba 0.1

Li 0.036

Si 6.03

S(6) 16.2

Cl 2.14

Alkalinity 363 as HCO3

water 1 # kg

SOLUTION 11 09-5-20

temp 13

pH 7 Calcite 0.627

pe 12.7

redox pe

units ppm

density 1

Ca 95

K 0.481

Mg 18.4

Na 4.47

Al 0.008

Sr 0.82

B 0.025

Ba 0.104

Li 0.035

Si 5.55

N(5) 0.052

S(6) 15.5

Cl 1.78

Alkalinity 376 as HCO3

water 1 # kg

SOLUTION 12 09-7-7

temp 13

pH 7 Calcite 0.406

pe 12.7

redox pe

units ppm

density 1

Ca 99.7

K 0.545

Mg 19.3

Na 4.82

Al 0.099

Sr 0.88

B 0.031

Ba 0.118

Li 0.038

Si 6.6

N(5) 0.043

S(6) 16.7

Cl 1.71

Alkalinity 402 as HCO3

water 1 # kg

SELECTED\_OUTPUT

file C:\Users\huan\Desktop\2008-09 3-5 selected.out.sel

reset false

ph true

pe true

temperature true

alkalinity true

ionic\_strength true

percent\_error true

molalities Ca+2 Mg+2

saturation\_indices CO2(g) Calcite Aragonite Dolomite

Quartz Chalcedony

-------------------------------------------

Beginning of initial solution calculations.

-------------------------------------------

Initial solution 1. 08-4-6

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 7.416e-008 7.416e-008

Alkalinity 5.722e-003 5.722e-003

B 1.851e-006 1.851e-006

Ba 6.556e-007 6.556e-007

Ca 2.189e-003 2.189e-003

Cl 6.462e-005 6.462e-005

K 2.131e-005 2.131e-005

Li 3.749e-006 3.749e-006

Mg 7.654e-004 7.654e-004

Na 1.850e-004 1.850e-004

S(6) 2.187e-004 2.187e-004

Si 7.710e-005 7.710e-005

Sr 8.906e-006 8.906e-006

----------------------------Description of solution----------------------------

pH = 7.958 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 408

Density (g/cm3) = 0.99978

Activity of water = 1.000

Ionic strength = 8.891e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 5.809e-003

Total CO2 (mol/kg) = 5.809e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -8.576e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.73

Iterations = 11

Total H = 1.110183e+002

Total O = 5.552468e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.804e-007 3.449e-007 -6.420 -6.462 -0.043

H+ 1.200e-008 1.102e-008 -7.921 -7.958 -0.037

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 7.416e-008

Al(OH)4- 7.363e-008 6.688e-008 -7.133 -7.175 -0.042

Al(OH)3 4.402e-010 4.411e-010 -9.356 -9.355 0.001

Al(OH)2+ 9.478e-011 8.610e-011 -10.023 -10.065 -0.042

AlOH+2 5.486e-013 3.735e-013 -12.261 -12.428 -0.167

Al+3 1.984e-015 9.236e-016 -14.702 -15.035 -0.332

AlSO4+ 3.333e-016 3.027e-016 -15.477 -15.519 -0.042

Al(SO4)2- 1.212e-018 1.101e-018 -17.916 -17.958 -0.042

AlHSO4+2 3.986e-025 2.714e-025 -24.399 -24.566 -0.167

B 1.851e-006

H3BO3 1.770e-006 1.774e-006 -5.752 -5.751 0.001

H2BO3- 8.113e-008 7.370e-008 -7.091 -7.133 -0.042

Ba 6.556e-007

Ba+2 6.121e-007 4.202e-007 -6.213 -6.377 -0.163

BaSO4 2.562e-008 2.567e-008 -7.591 -7.591 0.001

BaHCO3+ 1.520e-008 1.381e-008 -7.818 -7.860 -0.042

BaCO3 2.732e-009 2.738e-009 -8.563 -8.563 0.001

BaOH+ 1.422e-012 1.292e-012 -11.847 -11.889 -0.042

C(4) 5.809e-003

HCO3- 5.489e-003 5.001e-003 -2.261 -2.301 -0.040

CO2 1.500e-004 1.503e-004 -3.824 -3.823 0.001

CaHCO3+ 7.795e-005 7.102e-005 -4.108 -4.149 -0.040

CaCO3 3.164e-005 3.171e-005 -4.500 -4.499 0.001

MgHCO3+ 3.085e-005 2.803e-005 -4.511 -4.552 -0.042

CO3-2 2.328e-005 1.605e-005 -4.633 -4.795 -0.162

MgCO3 6.322e-006 6.334e-006 -5.199 -5.198 0.001

NaHCO3 4.705e-007 4.714e-007 -6.327 -6.327 0.001

SrHCO3+ 3.236e-007 2.948e-007 -6.490 -6.530 -0.040

SrCO3 4.169e-008 4.177e-008 -7.380 -7.379 0.001

NaCO3- 2.935e-008 2.666e-008 -7.532 -7.574 -0.042

BaHCO3+ 1.520e-008 1.381e-008 -7.818 -7.860 -0.042

BaCO3 2.732e-009 2.738e-009 -8.563 -8.563 0.001

Ca 2.189e-003

Ca+2 2.049e-003 1.412e-003 -2.688 -2.850 -0.162

CaHCO3+ 7.795e-005 7.102e-005 -4.108 -4.149 -0.040

CaCO3 3.164e-005 3.171e-005 -4.500 -4.499 0.001

CaSO4 3.048e-005 3.055e-005 -4.516 -4.515 0.001

CaOH+ 2.339e-008 2.125e-008 -7.631 -7.673 -0.042

CaHSO4+ 1.904e-012 1.729e-012 -11.720 -11.762 -0.042

Cl 6.462e-005

Cl- 6.462e-005 5.861e-005 -4.190 -4.232 -0.042

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -44.412 -44.411 0.001

K 2.131e-005

K+ 2.130e-005 1.932e-005 -4.672 -4.714 -0.042

KSO4- 1.464e-008 1.330e-008 -7.834 -7.876 -0.042

KOH 6.064e-012 6.076e-012 -11.217 -11.216 0.001

Li 3.749e-006

Li+ 3.747e-006 3.419e-006 -5.426 -5.466 -0.040

LiSO4- 2.003e-009 1.819e-009 -8.698 -8.740 -0.042

LiOH 7.090e-012 7.105e-012 -11.149 -11.148 0.001

Mg 7.654e-004

Mg+2 7.179e-004 4.974e-004 -3.144 -3.303 -0.159

MgHCO3+ 3.085e-005 2.803e-005 -4.511 -4.552 -0.042

MgSO4 1.028e-005 1.030e-005 -4.988 -4.987 0.001

MgCO3 6.322e-006 6.334e-006 -5.199 -5.198 0.001

MgOH+ 5.831e-008 5.297e-008 -7.234 -7.276 -0.042

Na 1.850e-004

Na+ 1.844e-004 1.676e-004 -3.734 -3.776 -0.041

NaHCO3 4.705e-007 4.714e-007 -6.327 -6.327 0.001

NaSO4- 1.041e-007 9.460e-008 -6.982 -7.024 -0.042

NaCO3- 2.935e-008 2.666e-008 -7.532 -7.574 -0.042

NaOH 1.003e-010 1.005e-010 -9.999 -9.998 0.001

O(0) 5.102e-008

O2 2.551e-008 2.556e-008 -7.593 -7.592 0.001

S(6) 2.187e-004

SO4-2 1.777e-004 1.219e-004 -3.750 -3.914 -0.164

CaSO4 3.048e-005 3.055e-005 -4.516 -4.515 0.001

MgSO4 1.028e-005 1.030e-005 -4.988 -4.987 0.001

SrSO4 1.190e-007 1.192e-007 -6.925 -6.924 0.001

NaSO4- 1.041e-007 9.460e-008 -6.982 -7.024 -0.042

BaSO4 2.562e-008 2.567e-008 -7.591 -7.591 0.001

KSO4- 1.464e-008 1.330e-008 -7.834 -7.876 -0.042

LiSO4- 2.003e-009 1.819e-009 -8.698 -8.740 -0.042

HSO4- 1.122e-010 1.019e-010 -9.950 -9.992 -0.042

CaHSO4+ 1.904e-012 1.729e-012 -11.720 -11.762 -0.042

AlSO4+ 3.333e-016 3.027e-016 -15.477 -15.519 -0.042

Al(SO4)2- 1.212e-018 1.101e-018 -17.916 -17.958 -0.042

AlHSO4+2 3.986e-025 2.714e-025 -24.399 -24.566 -0.167

Si 7.710e-005

H4SiO4 7.638e-005 7.654e-005 -4.117 -4.116 0.001

H3SiO4- 7.172e-007 6.515e-007 -6.144 -6.186 -0.042

H2SiO4-2 2.550e-012 1.737e-012 -11.593 -11.760 -0.167

Sr 8.906e-006

Sr+2 8.422e-006 5.812e-006 -5.075 -5.236 -0.161

SrHCO3+ 3.236e-007 2.948e-007 -6.490 -6.530 -0.040

SrSO4 1.190e-007 1.192e-007 -6.925 -6.924 0.001

SrCO3 4.169e-008 4.177e-008 -7.380 -7.379 0.001

SrOH+ 2.970e-011 2.704e-011 -10.527 -10.568 -0.041

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -2.78 8.84 11.61 Al(OH)3

Albite -4.50 -23.30 -18.80 NaAlSi3O8

Alunite -10.04 -9.90 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.43 -6.76 -4.33 CaSO4

Anorthite -5.36 -25.43 -20.07 CaAl2Si2O8

Aragonite 0.62 -7.64 -8.27 CaCO3

Barite -0.11 -10.29 -10.18 BaSO4

Ca-Montmorillonite -1.39 -48.21 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.78 -7.64 -8.42 CaCO3

Celestite -2.53 -9.15 -6.62 SrSO4

Chalcedony -0.42 -4.12 -3.70 SiO2

Chlorite(14A) -4.65 68.39 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -4.14 29.60 33.75 Mg3Si2O5(OH)4

CO2(g) -2.51 -3.82 -1.31 CO2

Dolomite 1.06 -15.74 -16.80 CaMg(CO3)2

Gibbsite 0.03 8.84 8.81 Al(OH)3

Gypsum -2.18 -6.76 -4.59 CaSO4:2H2O

H2(g) -41.32 -44.41 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.56 -8.01 1.55 NaCl

Illite -2.16 -44.11 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -2.72 -24.24 -21.52 KAlSi3O8

K-mica 2.88 17.41 14.53 KAl3Si3O10(OH)2

Kaolinite 0.93 9.45 8.52 Al2Si2O5(OH)4

O2(g) -4.80 -7.59 -2.79 O2

Quartz 0.05 -4.12 -4.16 SiO2

Sepiolite -3.21 12.88 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -5.78 12.88 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.30 -4.12 -2.81 SiO2

Strontianite -0.75 -10.03 -9.28 SrCO3

Talc -1.45 21.37 22.82 Mg3Si4O10(OH)2

Witherite -2.56 -11.17 -8.61 BaCO3

Initial solution 2. 08-5-20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 1.431e-005 1.431e-005

Alkalinity 5.952e-003 5.952e-003

B 2.221e-006 2.221e-006

Ba 7.285e-007 7.285e-007

Ca 2.307e-003 2.307e-003

Cl 7.168e-005 7.168e-005

K 2.259e-005 2.259e-005

Li 4.326e-006 4.326e-006

Mg 7.984e-004 7.984e-004

Na 1.871e-004 1.871e-004

S(6) 2.156e-004 2.156e-004

Si 9.958e-005 9.958e-005

Sr 9.249e-006 9.249e-006

----------------------------Description of solution----------------------------

pH = 7.767 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 424

Density (g/cm3) = 0.99980

Activity of water = 1.000

Ionic strength = 9.290e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.092e-003

Total CO2 (mol/kg) = 6.092e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = 3.196e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.26

Iterations = 11

Total H = 1.110187e+002

Total O = 5.552558e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.459e-007 2.225e-007 -6.609 -6.653 -0.043

H+ 1.863e-008 1.709e-008 -7.730 -7.767 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 1.431e-005

Al(OH)4- 1.414e-005 1.282e-005 -4.850 -4.892 -0.043

Al(OH)3 1.308e-007 1.311e-007 -6.883 -6.882 0.001

Al(OH)2+ 4.375e-008 3.967e-008 -7.359 -7.402 -0.043

AlOH+2 3.947e-010 2.668e-010 -9.404 -9.574 -0.170

Al+3 2.226e-012 1.023e-012 -11.652 -11.990 -0.338

AlSO4+ 3.591e-013 3.256e-013 -12.445 -12.487 -0.043

Al(SO4)2- 1.269e-015 1.150e-015 -14.897 -14.939 -0.043

AlHSO4+2 6.696e-022 4.526e-022 -21.174 -21.344 -0.170

B 2.221e-006

H3BO3 2.157e-006 2.162e-006 -5.666 -5.665 0.001

H2BO3- 6.392e-008 5.795e-008 -7.194 -7.237 -0.043

Ba 7.285e-007

Ba+2 6.815e-007 4.646e-007 -6.167 -6.333 -0.166

BaSO4 2.751e-008 2.757e-008 -7.561 -7.560 0.001

BaHCO3+ 1.742e-008 1.580e-008 -7.759 -7.801 -0.043

BaCO3 2.016e-009 2.021e-009 -8.695 -8.695 0.001

BaOH+ 1.016e-012 9.211e-013 -11.993 -12.036 -0.043

C(4) 6.092e-003

HCO3- 5.690e-003 5.176e-003 -2.245 -2.286 -0.041

CO2 2.407e-004 2.412e-004 -3.619 -3.618 0.001

CaHCO3+ 8.492e-005 7.724e-005 -4.071 -4.112 -0.041

MgHCO3+ 3.321e-005 3.011e-005 -4.479 -4.521 -0.043

CaCO3 2.220e-005 2.224e-005 -4.654 -4.653 0.001

CO3-2 1.565e-005 1.071e-005 -4.805 -4.970 -0.165

MgCO3 4.380e-006 4.390e-006 -5.358 -5.358 0.001

NaHCO3 4.917e-007 4.928e-007 -6.308 -6.307 0.001

SrHCO3+ 3.463e-007 3.150e-007 -6.461 -6.502 -0.041

SrCO3 2.872e-008 2.878e-008 -7.542 -7.541 0.001

NaCO3- 1.983e-008 1.798e-008 -7.703 -7.745 -0.043

BaHCO3+ 1.742e-008 1.580e-008 -7.759 -7.801 -0.043

BaCO3 2.016e-009 2.021e-009 -8.695 -8.695 0.001

Ca 2.307e-003

Ca+2 2.168e-003 1.483e-003 -2.664 -2.829 -0.165

CaHCO3+ 8.492e-005 7.724e-005 -4.071 -4.112 -0.041

CaSO4 3.111e-005 3.118e-005 -4.507 -4.506 0.001

CaCO3 2.220e-005 2.224e-005 -4.654 -4.653 0.001

CaOH+ 1.589e-008 1.440e-008 -7.799 -7.842 -0.043

CaHSO4+ 3.018e-012 2.736e-012 -11.520 -11.563 -0.043

Cl 7.168e-005

Cl- 7.168e-005 6.489e-005 -4.145 -4.188 -0.043

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -44.032 -44.031 0.001

K 2.259e-005

K+ 2.258e-005 2.044e-005 -4.646 -4.690 -0.043

KSO4- 1.508e-008 1.367e-008 -7.822 -7.864 -0.043

KOH 4.138e-012 4.147e-012 -11.383 -11.382 0.001

Li 4.326e-006

Li+ 4.323e-006 3.938e-006 -5.364 -5.405 -0.041

LiSO4- 2.245e-009 2.035e-009 -8.649 -8.691 -0.043

LiOH 5.268e-012 5.279e-012 -11.278 -11.277 0.001

Mg 7.984e-004

Mg+2 7.504e-004 5.163e-004 -3.125 -3.287 -0.162

MgHCO3+ 3.321e-005 3.011e-005 -4.479 -4.521 -0.043

MgSO4 1.036e-005 1.038e-005 -4.985 -4.984 0.001

MgCO3 4.380e-006 4.390e-006 -5.358 -5.358 0.001

MgOH+ 3.912e-008 3.547e-008 -7.408 -7.450 -0.043

Na 1.871e-004

Na+ 1.865e-004 1.693e-004 -3.729 -3.771 -0.042

NaHCO3 4.917e-007 4.928e-007 -6.308 -6.307 0.001

NaSO4- 1.024e-007 9.280e-008 -6.990 -7.032 -0.043

NaCO3- 1.983e-008 1.798e-008 -7.703 -7.745 -0.043

NaOH 6.531e-011 6.545e-011 -10.185 -10.184 0.001

O(0) 8.831e-009

O2 4.416e-009 4.425e-009 -8.355 -8.354 0.001

S(6) 2.156e-004

SO4-2 1.739e-004 1.184e-004 -3.760 -3.927 -0.167

CaSO4 3.111e-005 3.118e-005 -4.507 -4.506 0.001

MgSO4 1.036e-005 1.038e-005 -4.985 -4.984 0.001

SrSO4 1.193e-007 1.195e-007 -6.923 -6.923 0.001

NaSO4- 1.024e-007 9.280e-008 -6.990 -7.032 -0.043

BaSO4 2.751e-008 2.757e-008 -7.561 -7.560 0.001

KSO4- 1.508e-008 1.367e-008 -7.822 -7.864 -0.043

LiSO4- 2.245e-009 2.035e-009 -8.649 -8.691 -0.043

HSO4- 1.692e-010 1.534e-010 -9.772 -9.814 -0.043

CaHSO4+ 3.018e-012 2.736e-012 -11.520 -11.563 -0.043

AlSO4+ 3.591e-013 3.256e-013 -12.445 -12.487 -0.043

Al(SO4)2- 1.269e-015 1.150e-015 -14.897 -14.939 -0.043

AlHSO4+2 6.696e-022 4.526e-022 -21.174 -21.344 -0.170

Si 9.958e-005

H4SiO4 9.898e-005 9.919e-005 -4.004 -4.004 0.001

H3SiO4- 6.007e-007 5.446e-007 -6.221 -6.264 -0.043

H2SiO4-2 1.386e-012 9.364e-013 -11.858 -12.029 -0.170

Sr 9.249e-006

Sr+2 8.755e-006 5.999e-006 -5.058 -5.222 -0.164

SrHCO3+ 3.463e-007 3.150e-007 -6.461 -6.502 -0.041

SrSO4 1.193e-007 1.195e-007 -6.923 -6.923 0.001

SrCO3 2.872e-008 2.878e-008 -7.542 -7.541 0.001

SrOH+ 1.981e-011 1.800e-011 -10.703 -10.745 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -0.30 11.31 11.61 Al(OH)3

Albite -1.88 -20.67 -18.80 NaAlSi3O8

Alunite -2.05 -1.91 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.42 -6.76 -4.33 CaSO4

Anorthite -0.55 -20.62 -20.07 CaAl2Si2O8

Aragonite 0.47 -7.80 -8.27 CaCO3

Barite -0.08 -10.26 -10.18 BaSO4

Ca-Montmorillonite 4.73 -42.09 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.62 -7.80 -8.42 CaCO3

Celestite -2.52 -9.15 -6.62 SrSO4

Chalcedony -0.31 -4.00 -3.70 SiO2

Chlorite(14A) -1.19 71.85 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -5.01 28.74 33.75 Mg3Si2O5(OH)4

CO2(g) -2.30 -3.62 -1.31 CO2

Dolomite 0.74 -16.06 -16.80 CaMg(CO3)2

Gibbsite 2.50 11.31 8.81 Al(OH)3

Gypsum -2.17 -6.76 -4.59 CaSO4:2H2O

H2(g) -40.93 -44.03 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.51 -7.96 1.55 NaCl

Illite 3.73 -38.22 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -0.07 -21.59 -21.52 KAlSi3O8

K-mica 10.47 25.00 14.53 KAl3Si3O10(OH)2

Kaolinite 6.10 14.62 8.52 Al2Si2O5(OH)4

O2(g) -5.56 -8.35 -2.79 O2

Quartz 0.16 -4.00 -4.16 SiO2

Sepiolite -3.60 12.48 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -6.18 12.48 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.19 -4.00 -2.81 SiO2

Strontianite -0.91 -10.19 -9.28 SrCO3

Talc -2.09 20.73 22.82 Mg3Si4O10(OH)2

Witherite -2.69 -11.30 -8.61 BaCO3

Initial solution 3. 08-6-21

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 6.378e-003 6.378e-003

B 2.684e-006 2.684e-006

Ba 7.722e-007 7.722e-007

Ca 2.374e-003 2.374e-003

Cl 7.112e-005 7.112e-005

K 2.270e-005 2.270e-005

Li 4.614e-006 4.614e-006

Mg 8.148e-004 8.148e-004

N(5) 3.072e-006 3.072e-006

Na 2.072e-004 2.072e-004

S(6) 1.614e-004 1.614e-004

Si 9.642e-005 9.642e-005

Sr 9.592e-006 9.592e-006

----------------------------Description of solution----------------------------

pH = 7.573 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 442

Density (g/cm3) = 0.99982

Activity of water = 1.000

Ionic strength = 9.628e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.756e-003

Total CO2 (mol/kg) = 6.756e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -1.426e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.10

Iterations = 9

Total H = 1.110191e+002

Total O = 5.552713e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.575e-007 1.423e-007 -6.803 -6.847 -0.044

H+ 2.917e-008 2.672e-008 -7.535 -7.573 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 2.684e-006

H3BO3 2.634e-006 2.640e-006 -5.579 -5.578 0.001

H2BO3- 4.999e-008 4.526e-008 -7.301 -7.344 -0.043

Ba 7.722e-007

Ba+2 7.289e-007 4.939e-007 -6.137 -6.306 -0.169

BaSO4 2.169e-008 2.174e-008 -7.664 -7.663 0.001

BaHCO3+ 2.014e-008 1.823e-008 -7.696 -7.739 -0.043

BaCO3 1.488e-009 1.491e-009 -8.827 -8.826 0.001

BaOH+ 6.917e-013 6.262e-013 -12.160 -12.203 -0.043

C(4) 6.756e-003

HCO3- 6.186e-003 5.618e-003 -2.209 -2.250 -0.042

CO2 4.085e-004 4.094e-004 -3.389 -3.388 0.001

CaHCO3+ 9.479e-005 8.609e-005 -4.023 -4.065 -0.042

MgHCO3+ 3.670e-005 3.323e-005 -4.435 -4.478 -0.043

CaCO3 1.582e-005 1.586e-005 -4.801 -4.800 0.001

CO3-2 1.093e-005 7.437e-006 -4.961 -5.129 -0.167

MgCO3 3.091e-006 3.098e-006 -5.510 -5.509 0.001

NaHCO3 5.898e-007 5.912e-007 -6.229 -6.228 0.001

SrHCO3+ 3.886e-007 3.530e-007 -6.410 -6.452 -0.042

SrCO3 2.058e-008 2.063e-008 -7.686 -7.686 0.001

BaHCO3+ 2.014e-008 1.823e-008 -7.696 -7.739 -0.043

NaCO3- 1.523e-008 1.379e-008 -7.817 -7.860 -0.043

BaCO3 1.488e-009 1.491e-009 -8.827 -8.826 0.001

Ca 2.374e-003

Ca+2 2.240e-003 1.523e-003 -2.650 -2.817 -0.167

CaHCO3+ 9.479e-005 8.609e-005 -4.023 -4.065 -0.042

CaSO4 2.369e-005 2.375e-005 -4.625 -4.624 0.001

CaCO3 1.582e-005 1.586e-005 -4.801 -4.800 0.001

CaOH+ 1.045e-008 9.459e-009 -7.981 -8.024 -0.043

CaHSO4+ 3.600e-012 3.259e-012 -11.444 -11.487 -0.043

Cl 7.112e-005

Cl- 7.112e-005 6.427e-005 -4.148 -4.192 -0.044

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.643 -43.642 0.001

K 2.270e-005

K+ 2.269e-005 2.050e-005 -4.644 -4.688 -0.044

KSO4- 1.123e-008 1.017e-008 -7.949 -7.993 -0.043

KOH 2.654e-012 2.660e-012 -11.576 -11.575 0.001

Li 4.614e-006

Li+ 4.612e-006 4.196e-006 -5.336 -5.377 -0.041

LiSO4- 1.777e-009 1.608e-009 -8.750 -8.794 -0.043

LiOH 3.589e-012 3.597e-012 -11.445 -11.444 0.001

Mg 8.148e-004

Mg+2 7.672e-004 5.249e-004 -3.115 -3.280 -0.165

MgHCO3+ 3.670e-005 3.323e-005 -4.435 -4.478 -0.043

MgSO4 7.814e-006 7.831e-006 -5.107 -5.106 0.001

MgCO3 3.091e-006 3.098e-006 -5.510 -5.509 0.001

MgOH+ 2.547e-008 2.306e-008 -7.594 -7.637 -0.043

N(5) 3.072e-006

NO3- 3.072e-006 2.771e-006 -5.513 -5.557 -0.045

Na 2.072e-004

Na+ 2.065e-004 1.871e-004 -3.685 -3.728 -0.043

NaHCO3 5.898e-007 5.912e-007 -6.229 -6.228 0.001

NaSO4- 8.404e-008 7.608e-008 -7.076 -7.119 -0.043

NaCO3- 1.523e-008 1.379e-008 -7.817 -7.860 -0.043

NaOH 4.616e-011 4.626e-011 -10.336 -10.335 0.001

O(0) 1.477e-009

O2 7.386e-010 7.402e-010 -9.132 -9.131 0.001

S(6) 1.614e-004

SO4-2 1.297e-004 8.782e-005 -3.887 -4.056 -0.169

CaSO4 2.369e-005 2.375e-005 -4.625 -4.624 0.001

MgSO4 7.814e-006 7.831e-006 -5.107 -5.106 0.001

SrSO4 9.133e-008 9.154e-008 -7.039 -7.038 0.001

NaSO4- 8.404e-008 7.608e-008 -7.076 -7.119 -0.043

BaSO4 2.169e-008 2.174e-008 -7.664 -7.663 0.001

KSO4- 1.123e-008 1.017e-008 -7.949 -7.993 -0.043

LiSO4- 1.777e-009 1.608e-009 -8.750 -8.794 -0.043

HSO4- 1.966e-010 1.780e-010 -9.706 -9.750 -0.043

CaHSO4+ 3.600e-012 3.259e-012 -11.444 -11.487 -0.043

Si 9.642e-005

H4SiO4 9.604e-005 9.626e-005 -4.018 -4.017 0.001

H3SiO4- 3.734e-007 3.380e-007 -6.428 -6.471 -0.043

H2SiO4-2 5.533e-013 3.717e-013 -12.257 -12.430 -0.173

Sr 9.592e-006

Sr+2 9.091e-006 6.194e-006 -5.041 -5.208 -0.167

SrHCO3+ 3.886e-007 3.530e-007 -6.410 -6.452 -0.042

SrSO4 9.133e-008 9.154e-008 -7.039 -7.038 0.001

SrCO3 2.058e-008 2.063e-008 -7.686 -7.686 0.001

SrOH+ 1.310e-011 1.189e-011 -10.883 -10.925 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.54 -6.87 -4.33 CaSO4

Aragonite 0.32 -7.95 -8.27 CaCO3

Barite -0.18 -10.36 -10.18 BaSO4

Calcite 0.48 -7.95 -8.42 CaCO3

Celestite -2.64 -9.26 -6.62 SrSO4

Chalcedony -0.32 -4.02 -3.70 SiO2

Chrysotile -6.18 27.57 33.75 Mg3Si2O5(OH)4

CO2(g) -2.07 -3.39 -1.31 CO2

Dolomite 0.45 -16.35 -16.80 CaMg(CO3)2

Gypsum -2.29 -6.87 -4.59 CaSO4:2H2O

H2(g) -40.55 -43.64 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.47 -7.92 1.55 NaCl

O2(g) -6.34 -9.13 -2.79 O2

Quartz 0.15 -4.02 -4.16 SiO2

Sepiolite -4.41 11.68 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -6.98 11.68 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.20 -4.02 -2.81 SiO2

Strontianite -1.06 -10.34 -9.28 SrCO3

Talc -3.29 19.53 22.82 Mg3Si4O10(OH)2

Witherite -2.82 -11.43 -8.61 BaCO3

Initial solution 4. 08-8-7

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 2.225e-007 2.225e-007

Alkalinity 6.428e-003 6.428e-003

B 3.239e-006 3.239e-006

Ba 8.159e-007 8.159e-007

Ca 2.374e-003 2.374e-003

Cl 6.717e-005 6.717e-005

K 2.423e-005 2.423e-005

Li 4.902e-006 4.902e-006

Mg 7.984e-004 7.984e-004

N(5) 3.429e-006 3.429e-006

Na 1.906e-004 1.906e-004

S(6) 1.708e-004 1.708e-004

Si 1.044e-004 1.044e-004

Sr 9.820e-006 9.820e-006

----------------------------Description of solution----------------------------

pH = 7.363 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 443

Density (g/cm3) = 0.99982

Activity of water = 1.000

Ionic strength = 9.638e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.079e-003

Total CO2 (mol/kg) = 7.079e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -2.534e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.95

Iterations = 11

Total H = 1.110193e+002

Total O = 5.552790e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 9.701e-008 8.764e-008 -7.013 -7.057 -0.044

H+ 4.735e-008 4.338e-008 -7.325 -7.363 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 2.225e-007

Al(OH)4- 2.131e-007 1.930e-007 -6.671 -6.715 -0.043

Al(OH)3 4.997e-009 5.009e-009 -8.301 -8.300 0.001

Al(OH)2+ 4.251e-009 3.848e-009 -8.372 -8.415 -0.043

AlOH+2 9.783e-011 6.570e-011 -10.010 -10.182 -0.173

Al+3 1.407e-012 6.394e-013 -11.852 -12.194 -0.343

AlSO4+ 1.766e-013 1.599e-013 -12.753 -12.796 -0.043

Al(SO4)2- 4.899e-016 4.435e-016 -15.310 -15.353 -0.043

AlHSO4+2 8.399e-022 5.641e-022 -21.076 -21.249 -0.173

B 3.239e-006

H3BO3 3.202e-006 3.209e-006 -5.495 -5.494 0.001

H2BO3- 3.743e-008 3.389e-008 -7.427 -7.470 -0.043

Ba 8.159e-007

Ba+2 7.692e-007 5.211e-007 -6.114 -6.283 -0.169

BaSO4 2.423e-008 2.428e-008 -7.616 -7.615 0.001

BaHCO3+ 2.149e-008 1.945e-008 -7.668 -7.711 -0.043

BaCO3 9.779e-010 9.801e-010 -9.010 -9.009 0.001

BaOH+ 4.496e-013 4.070e-013 -12.347 -12.390 -0.043

C(4) 7.079e-003

HCO3- 6.256e-003 5.682e-003 -2.204 -2.246 -0.042

CO2 6.707e-004 6.722e-004 -3.173 -3.173 0.001

CaHCO3+ 9.599e-005 8.718e-005 -4.018 -4.060 -0.042

MgHCO3+ 3.638e-005 3.293e-005 -4.439 -4.482 -0.043

CaCO3 9.868e-006 9.890e-006 -5.006 -5.005 0.001

CO3-2 6.809e-006 4.632e-006 -5.167 -5.334 -0.167

MgCO3 1.887e-006 1.891e-006 -5.724 -5.723 0.001

NaHCO3 5.489e-007 5.501e-007 -6.261 -6.260 0.001

SrHCO3+ 4.023e-007 3.653e-007 -6.396 -6.437 -0.042

BaHCO3+ 2.149e-008 1.945e-008 -7.668 -7.711 -0.043

SrCO3 1.312e-008 1.315e-008 -7.882 -7.881 0.001

NaCO3- 8.732e-009 7.905e-009 -8.059 -8.102 -0.043

BaCO3 9.779e-010 9.801e-010 -9.010 -9.009 0.001

Ca 2.374e-003

Ca+2 2.243e-003 1.525e-003 -2.649 -2.817 -0.168

CaHCO3+ 9.599e-005 8.718e-005 -4.018 -4.060 -0.042

CaSO4 2.512e-005 2.517e-005 -4.600 -4.599 0.001

CaCO3 9.868e-006 9.890e-006 -5.006 -5.005 0.001

CaOH+ 6.444e-009 5.834e-009 -8.191 -8.234 -0.043

CaHSO4+ 6.196e-012 5.609e-012 -11.208 -11.251 -0.043

Cl 6.717e-005

Cl- 6.717e-005 6.070e-005 -4.173 -4.217 -0.044

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.222 -43.221 0.001

K 2.423e-005

K+ 2.422e-005 2.189e-005 -4.616 -4.660 -0.044

KSO4- 1.270e-008 1.150e-008 -7.896 -7.939 -0.043

KOH 1.745e-012 1.749e-012 -11.758 -11.757 0.001

Li 4.902e-006

Li+ 4.900e-006 4.458e-006 -5.310 -5.351 -0.041

LiSO4- 1.998e-009 1.809e-009 -8.699 -8.743 -0.043

LiOH 2.348e-012 2.354e-012 -11.629 -11.628 0.001

Mg 7.984e-004

Mg+2 7.520e-004 5.144e-004 -3.124 -3.289 -0.165

MgHCO3+ 3.638e-005 3.293e-005 -4.439 -4.482 -0.043

MgSO4 8.107e-006 8.125e-006 -5.091 -5.090 0.001

MgCO3 1.887e-006 1.891e-006 -5.724 -5.723 0.001

MgOH+ 1.538e-008 1.392e-008 -7.813 -7.856 -0.043

N(5) 3.429e-006

NO3- 3.429e-006 3.093e-006 -5.465 -5.510 -0.045

Na 1.906e-004

Na+ 1.900e-004 1.722e-004 -3.721 -3.764 -0.043

NaHCO3 5.489e-007 5.501e-007 -6.261 -6.260 0.001

NaSO4- 8.187e-008 7.411e-008 -7.087 -7.130 -0.043

NaCO3- 8.732e-009 7.905e-009 -8.059 -8.102 -0.043

NaOH 2.616e-011 2.622e-011 -10.582 -10.581 0.001

O(0) 2.126e-010

O2 1.063e-010 1.065e-010 -9.973 -9.972 0.001

S(6) 1.708e-004

SO4-2 1.374e-004 9.298e-005 -3.862 -4.032 -0.170

CaSO4 2.512e-005 2.517e-005 -4.600 -4.599 0.001

MgSO4 8.107e-006 8.125e-006 -5.091 -5.090 0.001

SrSO4 9.897e-008 9.919e-008 -7.005 -7.004 0.001

NaSO4- 8.187e-008 7.411e-008 -7.087 -7.130 -0.043

BaSO4 2.423e-008 2.428e-008 -7.616 -7.615 0.001

KSO4- 1.270e-008 1.150e-008 -7.896 -7.939 -0.043

LiSO4- 1.998e-009 1.809e-009 -8.699 -8.743 -0.043

HSO4- 3.379e-010 3.059e-010 -9.471 -9.514 -0.043

CaHSO4+ 6.196e-012 5.609e-012 -11.208 -11.251 -0.043

AlSO4+ 1.766e-013 1.599e-013 -12.753 -12.796 -0.043

Al(SO4)2- 4.899e-016 4.435e-016 -15.310 -15.353 -0.043

AlHSO4+2 8.399e-022 5.641e-022 -21.076 -21.249 -0.173

Si 1.044e-004

H4SiO4 1.042e-004 1.044e-004 -3.982 -3.981 0.001

H3SiO4- 2.494e-007 2.258e-007 -6.603 -6.646 -0.043

H2SiO4-2 2.277e-013 1.529e-013 -12.643 -12.816 -0.173

Sr 9.820e-006

Sr+2 9.306e-006 6.339e-006 -5.031 -5.198 -0.167

SrHCO3+ 4.023e-007 3.653e-007 -6.396 -6.437 -0.042

SrSO4 9.897e-008 9.919e-008 -7.005 -7.004 0.001

SrCO3 1.312e-008 1.315e-008 -7.882 -7.881 0.001

SrOH+ 8.259e-012 7.493e-012 -11.083 -11.125 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -1.72 9.89 11.61 Al(OH)3

Albite -3.62 -22.42 -18.80 NaAlSi3O8

Alunite -5.27 -5.13 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.51 -6.85 -4.33 CaSO4

Anorthite -4.14 -24.21 -20.07 CaAl2Si2O8

Aragonite 0.12 -8.15 -8.27 CaCO3

Barite -0.13 -10.31 -10.18 BaSO4

Ca-Montmorillonite 1.38 -45.45 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.27 -8.15 -8.42 CaCO3

Celestite -2.61 -9.23 -6.62 SrSO4

Chalcedony -0.28 -3.98 -3.70 SiO2

Chlorite(14A) -8.01 65.03 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -7.40 26.35 33.75 Mg3Si2O5(OH)4

CO2(g) -1.86 -3.17 -1.31 CO2

Dolomite 0.03 -16.77 -16.80 CaMg(CO3)2

Gibbsite 1.08 9.89 8.81 Al(OH)3

Gypsum -2.26 -6.85 -4.59 CaSO4:2H2O

H2(g) -40.13 -43.22 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.53 -7.98 1.55 NaCl

Illite 0.12 -41.83 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -1.80 -23.32 -21.52 KAlSi3O8

K-mica 5.91 20.44 14.53 KAl3Si3O10(OH)2

Kaolinite 3.31 11.83 8.52 Al2Si2O5(OH)4

O2(g) -7.18 -9.97 -2.79 O2

Quartz 0.18 -3.98 -4.16 SiO2

Sepiolite -5.16 10.93 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -7.73 10.93 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.17 -3.98 -2.81 SiO2

Strontianite -1.25 -10.53 -9.28 SrCO3

Talc -4.44 18.39 22.82 Mg3Si4O10(OH)2

Witherite -3.01 -11.62 -8.61 BaCO3

Initial solution 5. 08-9-21

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 6.149e-003 6.149e-003

B 2.962e-006 2.962e-006

Ba 8.523e-007 8.523e-007

Ca 2.264e-003 2.264e-003

Cl 6.237e-005 6.237e-005

K 2.441e-005 2.441e-005

Li 6.633e-006 6.633e-006

Mg 7.531e-004 7.531e-004

N(5) 3.429e-006 3.429e-006

Na 1.937e-004 1.937e-004

S(6) 1.573e-004 1.573e-004

Si 1.011e-004 1.011e-004

Sr 9.592e-006 9.592e-006

----------------------------Description of solution----------------------------

pH = 7.285 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 424

Density (g/cm3) = 0.99980

Activity of water = 1.000

Ionic strength = 9.203e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.904e-003

Total CO2 (mol/kg) = 6.904e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -2.490e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.01

Iterations = 9

Total H = 1.110190e+002

Total O = 5.552721e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.102e-008 7.335e-008 -7.091 -7.135 -0.043

H+ 5.649e-008 5.183e-008 -7.248 -7.285 -0.037

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 2.962e-006

H3BO3 2.933e-006 2.939e-006 -5.533 -5.532 0.001

H2BO3- 2.864e-008 2.597e-008 -7.543 -7.585 -0.042

Ba 8.523e-007

Ba+2 8.059e-007 5.502e-007 -6.094 -6.260 -0.166

BaSO4 2.388e-008 2.393e-008 -7.622 -7.621 0.001

BaHCO3+ 2.174e-008 1.972e-008 -7.663 -7.705 -0.042

BaCO3 8.298e-010 8.316e-010 -9.081 -9.080 0.001

BaOH+ 3.964e-013 3.596e-013 -12.402 -12.444 -0.042

C(4) 6.904e-003

HCO3- 5.997e-003 5.456e-003 -2.222 -2.263 -0.041

CO2 7.697e-004 7.713e-004 -3.114 -3.113 0.001

CaHCO3+ 8.867e-005 8.068e-005 -4.052 -4.093 -0.041

MgHCO3+ 3.322e-005 3.013e-005 -4.479 -4.521 -0.042

CaCO3 7.643e-006 7.659e-006 -5.117 -5.116 0.001

CO3-2 5.431e-006 3.723e-006 -5.265 -5.429 -0.164

MgCO3 1.445e-006 1.448e-006 -5.840 -5.839 0.001

NaHCO3 5.367e-007 5.378e-007 -6.270 -6.269 0.001

SrHCO3+ 3.803e-007 3.460e-007 -6.420 -6.461 -0.041

BaHCO3+ 2.174e-008 1.972e-008 -7.663 -7.705 -0.042

SrCO3 1.040e-008 1.042e-008 -7.983 -7.982 0.001

NaCO3- 7.131e-009 6.468e-009 -8.147 -8.189 -0.042

BaCO3 8.298e-010 8.316e-010 -9.081 -9.080 0.001

Ca 2.264e-003

Ca+2 2.145e-003 1.470e-003 -2.669 -2.833 -0.164

CaHCO3+ 8.867e-005 8.068e-005 -4.052 -4.093 -0.041

CaSO4 2.260e-005 2.265e-005 -4.646 -4.645 0.001

CaCO3 7.643e-006 7.659e-006 -5.117 -5.116 0.001

CaOH+ 5.187e-009 4.705e-009 -8.285 -8.327 -0.042

CaHSO4+ 6.647e-012 6.029e-012 -11.177 -11.220 -0.042

Cl 6.237e-005

Cl- 6.237e-005 5.648e-005 -4.205 -4.248 -0.043

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.068 -43.067 0.001

K 2.441e-005

K+ 2.440e-005 2.210e-005 -4.613 -4.656 -0.043

KSO4- 1.194e-008 1.083e-008 -7.923 -7.965 -0.042

KOH 1.475e-012 1.478e-012 -11.831 -11.830 0.001

Li 6.633e-006

Li+ 6.630e-006 6.042e-006 -5.178 -5.219 -0.040

LiSO4- 2.524e-009 2.289e-009 -8.598 -8.640 -0.042

LiOH 2.664e-012 2.670e-012 -11.574 -11.574 0.001

Mg 7.531e-004

Mg+2 7.112e-004 4.901e-004 -3.148 -3.310 -0.162

MgHCO3+ 3.322e-005 3.013e-005 -4.479 -4.521 -0.042

MgSO4 7.211e-006 7.226e-006 -5.142 -5.141 0.001

MgCO3 1.445e-006 1.448e-006 -5.840 -5.839 0.001

MgOH+ 1.224e-008 1.110e-008 -7.912 -7.955 -0.042

N(5) 3.429e-006

NO3- 3.429e-006 3.100e-006 -5.465 -5.509 -0.044

Na 1.937e-004

Na+ 1.930e-004 1.753e-004 -3.714 -3.756 -0.042

NaHCO3 5.367e-007 5.378e-007 -6.270 -6.269 0.001

NaSO4- 7.766e-008 7.044e-008 -7.110 -7.152 -0.042

NaCO3- 7.131e-009 6.468e-009 -8.147 -8.189 -0.042

NaOH 2.229e-011 2.234e-011 -10.652 -10.651 0.001

O(0) 1.043e-010

O2 5.215e-011 5.226e-011 -10.283 -10.282 0.001

S(6) 1.573e-004

SO4-2 1.273e-004 8.680e-005 -3.895 -4.061 -0.166

CaSO4 2.260e-005 2.265e-005 -4.646 -4.645 0.001

MgSO4 7.211e-006 7.226e-006 -5.142 -5.141 0.001

SrSO4 9.113e-008 9.132e-008 -7.040 -7.039 0.001

NaSO4- 7.766e-008 7.044e-008 -7.110 -7.152 -0.042

BaSO4 2.388e-008 2.393e-008 -7.622 -7.621 0.001

KSO4- 1.194e-008 1.083e-008 -7.923 -7.965 -0.042

LiSO4- 2.524e-009 2.289e-009 -8.598 -8.640 -0.042

HSO4- 3.762e-010 3.412e-010 -9.425 -9.467 -0.042

CaHSO4+ 6.647e-012 6.029e-012 -11.177 -11.220 -0.042

Si 1.011e-004

H4SiO4 1.009e-004 1.011e-004 -3.996 -3.995 0.001

H3SiO4- 2.017e-007 1.830e-007 -6.695 -6.738 -0.042

H2SiO4-2 1.532e-013 1.037e-013 -12.815 -12.984 -0.169

Sr 9.592e-006

Sr+2 9.110e-006 6.252e-006 -5.040 -5.204 -0.164

SrHCO3+ 3.803e-007 3.460e-007 -6.420 -6.461 -0.041

SrSO4 9.113e-008 9.132e-008 -7.040 -7.039 0.001

SrCO3 1.040e-008 1.042e-008 -7.983 -7.982 0.001

SrOH+ 6.804e-012 6.185e-012 -11.167 -11.209 -0.041

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.56 -6.89 -4.33 CaSO4

Aragonite 0.01 -8.26 -8.27 CaCO3

Barite -0.14 -10.32 -10.18 BaSO4

Calcite 0.16 -8.26 -8.42 CaCO3

Celestite -2.64 -9.27 -6.62 SrSO4

Chalcedony -0.30 -4.00 -3.70 SiO2

Chrysotile -7.96 25.79 33.75 Mg3Si2O5(OH)4

CO2(g) -1.80 -3.11 -1.31 CO2

Dolomite -0.20 -17.00 -16.80 CaMg(CO3)2

Gypsum -2.31 -6.89 -4.59 CaSO4:2H2O

H2(g) -39.97 -43.07 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.56 -8.00 1.55 NaCl

O2(g) -7.49 -10.28 -2.79 O2

Quartz 0.17 -4.00 -4.16 SiO2

Sepiolite -5.55 10.54 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.12 10.54 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.18 -4.00 -2.81 SiO2

Strontianite -1.35 -10.63 -9.28 SrCO3

Talc -5.02 17.80 22.82 Mg3Si4O10(OH)2

Witherite -3.08 -11.69 -8.61 BaCO3

Initial solution 6. 08-11-2

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 4.709e-006 4.709e-006

Alkalinity 6.165e-003 6.165e-003

B 2.406e-006 2.406e-006

Ba 8.159e-007 8.159e-007

Ca 2.304e-003 2.304e-003

Cl 4.233e-005 4.233e-005

K 2.334e-005 2.334e-005

Li 4.181e-006 4.181e-006

Mg 7.901e-004 7.901e-004

N(5) 2.214e-006 2.214e-006

Na 1.958e-004 1.958e-004

S(6) 2.125e-004 2.125e-004

Si 1.032e-004 1.032e-004

Sr 9.934e-006 9.934e-006

----------------------------Description of solution----------------------------

pH = 7.322 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 431

Density (g/cm3) = 0.99981

Activity of water = 1.000

Ionic strength = 9.407e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.837e-003

Total CO2 (mol/kg) = 6.837e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -1.872e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.49

Iterations = 11

Total H = 1.110190e+002

Total O = 5.552732e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.818e-008 7.975e-008 -7.055 -7.098 -0.044

H+ 5.200e-008 4.767e-008 -7.284 -7.322 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 4.709e-006

Al(OH)4- 4.483e-006 4.063e-006 -5.348 -5.391 -0.043

Al(OH)3 1.156e-007 1.159e-007 -6.937 -6.936 0.001

Al(OH)2+ 1.080e-007 9.784e-008 -6.967 -7.009 -0.043

AlOH+2 2.722e-009 1.836e-009 -8.565 -8.736 -0.171

Al+3 4.290e-011 1.964e-011 -10.368 -10.707 -0.339

AlSO4+ 6.789e-012 6.152e-012 -11.168 -11.211 -0.043

Al(SO4)2- 2.360e-014 2.139e-014 -13.627 -13.670 -0.043

AlHSO4+2 3.537e-020 2.386e-020 -19.451 -19.622 -0.171

B 2.406e-006

H3BO3 2.381e-006 2.386e-006 -5.623 -5.622 0.001

H2BO3- 2.530e-008 2.293e-008 -7.597 -7.640 -0.043

Ba 8.159e-007

Ba+2 7.643e-007 5.198e-007 -6.117 -6.284 -0.167

BaSO4 3.029e-008 3.036e-008 -7.519 -7.518 0.001

BaHCO3+ 2.052e-008 1.860e-008 -7.688 -7.731 -0.043

BaCO3 8.508e-010 8.526e-010 -9.070 -9.069 0.001

BaOH+ 4.077e-013 3.694e-013 -12.390 -12.432 -0.043

C(4) 6.837e-003

HCO3- 5.989e-003 5.445e-003 -2.223 -2.264 -0.041

CO2 7.064e-004 7.079e-004 -3.151 -3.150 0.001

CaHCO3+ 8.949e-005 8.136e-005 -4.048 -4.090 -0.041

MgHCO3+ 3.458e-005 3.134e-005 -4.461 -4.504 -0.043

CaCO3 8.380e-006 8.398e-006 -5.077 -5.076 0.001

CO3-2 5.914e-006 4.040e-006 -5.228 -5.394 -0.166

MgCO3 1.634e-006 1.638e-006 -5.787 -5.786 0.001

NaHCO3 5.410e-007 5.422e-007 -6.267 -6.266 0.001

SrHCO3+ 3.908e-007 3.553e-007 -6.408 -6.449 -0.041

BaHCO3+ 2.052e-008 1.860e-008 -7.688 -7.731 -0.043

SrCO3 1.161e-008 1.164e-008 -7.935 -7.934 0.001

NaCO3- 7.823e-009 7.089e-009 -8.107 -8.149 -0.043

BaCO3 8.508e-010 8.526e-010 -9.070 -9.069 0.001

Ca 2.304e-003

Ca+2 2.176e-003 1.485e-003 -2.662 -2.828 -0.166

CaHCO3+ 8.949e-005 8.136e-005 -4.048 -4.090 -0.041

CaSO4 3.065e-005 3.072e-005 -4.514 -4.513 0.001

CaCO3 8.380e-006 8.398e-006 -5.077 -5.076 0.001

CaOH+ 5.704e-009 5.169e-009 -8.244 -8.287 -0.043

CaHSO4+ 8.301e-012 7.522e-012 -11.081 -11.124 -0.043

Cl 4.233e-005

Cl- 4.233e-005 3.830e-005 -4.373 -4.417 -0.043

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.140 -43.139 0.001

K 2.334e-005

K+ 2.332e-005 2.110e-005 -4.632 -4.676 -0.043

KSO4- 1.532e-008 1.389e-008 -7.815 -7.857 -0.043

KOH 1.531e-012 1.534e-012 -11.815 -11.814 0.001

Li 4.181e-006

Li+ 4.179e-006 3.805e-006 -5.379 -5.420 -0.041

LiSO4- 2.136e-009 1.935e-009 -8.670 -8.713 -0.043

LiOH 1.824e-012 1.828e-012 -11.739 -11.738 0.001

Mg 7.901e-004

Mg+2 7.438e-004 5.108e-004 -3.129 -3.292 -0.163

MgHCO3+ 3.458e-005 3.134e-005 -4.461 -4.504 -0.043

MgSO4 1.009e-005 1.011e-005 -4.996 -4.995 0.001

MgCO3 1.634e-006 1.638e-006 -5.787 -5.786 0.001

MgOH+ 1.388e-008 1.258e-008 -7.858 -7.900 -0.043

N(5) 2.214e-006

NO3- 2.214e-006 2.000e-006 -5.655 -5.699 -0.044

Na 1.958e-004

Na+ 1.952e-004 1.771e-004 -3.710 -3.752 -0.042

NaHCO3 5.410e-007 5.422e-007 -6.267 -6.266 0.001

NaSO4- 1.054e-007 9.552e-008 -6.977 -7.020 -0.043

NaCO3- 7.823e-009 7.089e-009 -8.107 -8.149 -0.043

NaOH 2.448e-011 2.454e-011 -10.611 -10.610 0.001

O(0) 1.458e-010

O2 7.288e-011 7.304e-011 -10.137 -10.136 0.001

S(6) 2.125e-004

SO4-2 1.714e-004 1.165e-004 -3.766 -3.934 -0.168

CaSO4 3.065e-005 3.072e-005 -4.514 -4.513 0.001

MgSO4 1.009e-005 1.011e-005 -4.996 -4.995 0.001

SrSO4 1.259e-007 1.261e-007 -6.900 -6.899 0.001

NaSO4- 1.054e-007 9.552e-008 -6.977 -7.020 -0.043

BaSO4 3.029e-008 3.036e-008 -7.519 -7.518 0.001

KSO4- 1.532e-008 1.389e-008 -7.815 -7.857 -0.043

LiSO4- 2.136e-009 1.935e-009 -8.670 -8.713 -0.043

HSO4- 4.649e-010 4.213e-010 -9.333 -9.375 -0.043

CaHSO4+ 8.301e-012 7.522e-012 -11.081 -11.124 -0.043

AlSO4+ 6.789e-012 6.152e-012 -11.168 -11.211 -0.043

Al(SO4)2- 2.360e-014 2.139e-014 -13.627 -13.670 -0.043

AlHSO4+2 3.537e-020 2.386e-020 -19.451 -19.622 -0.171

Si 1.032e-004

H4SiO4 1.030e-004 1.032e-004 -3.987 -3.986 0.001

H3SiO4- 2.242e-007 2.032e-007 -6.649 -6.692 -0.043

H2SiO4-2 1.857e-013 1.252e-013 -12.731 -12.902 -0.171

Sr 9.934e-006

Sr+2 9.406e-006 6.432e-006 -5.027 -5.192 -0.165

SrHCO3+ 3.908e-007 3.553e-007 -6.408 -6.449 -0.041

SrSO4 1.259e-007 1.261e-007 -6.900 -6.899 0.001

SrCO3 1.161e-008 1.164e-008 -7.935 -7.934 0.001

SrOH+ 7.619e-012 6.919e-012 -11.118 -11.160 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -0.36 11.26 11.61 Al(OH)3

Albite -2.30 -21.10 -18.80 NaAlSi3O8

Alunite -0.88 -0.73 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.43 -6.76 -4.33 CaSO4

Anorthite -1.51 -21.58 -20.07 CaAl2Si2O8

Aragonite 0.05 -8.22 -8.27 CaCO3

Barite -0.03 -10.22 -10.18 BaSO4

Ca-Montmorillonite 4.52 -42.30 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.20 -8.22 -8.42 CaCO3

Celestite -2.50 -9.13 -6.62 SrSO4

Chalcedony -0.29 -3.99 -3.70 SiO2

Chlorite(14A) -5.72 67.32 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -7.67 26.08 33.75 Mg3Si2O5(OH)4

CO2(g) -1.84 -3.15 -1.31 CO2

Dolomite -0.11 -16.91 -16.80 CaMg(CO3)2

Gibbsite 2.45 11.26 8.81 Al(OH)3

Gypsum -2.18 -6.76 -4.59 CaSO4:2H2O

H2(g) -40.04 -43.14 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.72 -8.17 1.55 NaCl

Illite 3.18 -38.76 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -0.50 -22.02 -21.52 KAlSi3O8

K-mica 9.93 24.46 14.53 KAl3Si3O10(OH)2

Kaolinite 6.02 14.54 8.52 Al2Si2O5(OH)4

O2(g) -7.34 -10.14 -2.79 O2

Quartz 0.18 -3.99 -4.16 SiO2

Sepiolite -5.34 10.75 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -7.91 10.75 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.17 -3.99 -2.81 SiO2

Strontianite -1.31 -10.59 -9.28 SrCO3

Talc -4.71 18.11 22.82 Mg3Si4O10(OH)2

Witherite -3.07 -11.68 -8.61 BaCO3

Initial solution 7. 08-11-30

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 7.416e-006 7.416e-006

Alkalinity 5.985e-003 5.985e-003

B 2.221e-006 2.221e-006

Ba 7.722e-007 7.722e-007

Ca 2.307e-003 2.307e-003

Cl 7.309e-005 7.309e-005

K 2.198e-005 2.198e-005

Li 6.056e-006 6.056e-006

Mg 7.613e-004 7.613e-004

N(5) 4.857e-006 4.857e-006

Na 1.845e-004 1.845e-004

S(6) 2.281e-004 2.281e-004

Si 9.825e-005 9.825e-005

Sr 9.592e-006 9.592e-006

----------------------------Description of solution----------------------------

pH = 7.469 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 426

Density (g/cm3) = 0.99980

Activity of water = 1.000

Ionic strength = 9.292e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.420e-003

Total CO2 (mol/kg) = 6.420e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -1.276e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.03

Iterations = 10

Total H = 1.110188e+002

Total O = 5.552635e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.238e-007 1.120e-007 -6.907 -6.951 -0.043

H+ 3.701e-008 3.394e-008 -7.432 -7.469 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 7.416e-006

Al(OH)4- 7.195e-006 6.523e-006 -5.143 -5.186 -0.043

Al(OH)3 1.322e-007 1.325e-007 -6.879 -6.878 0.001

Al(OH)2+ 8.784e-008 7.964e-008 -7.056 -7.099 -0.043

AlOH+2 1.574e-009 1.064e-009 -8.803 -8.973 -0.170

Al+3 1.764e-011 8.102e-012 -10.754 -11.091 -0.338

AlSO4+ 3.015e-012 2.734e-012 -11.521 -11.563 -0.043

Al(SO4)2- 1.129e-014 1.024e-014 -13.947 -13.990 -0.043

AlHSO4+2 1.117e-020 7.548e-021 -19.952 -20.122 -0.170

B 2.221e-006

H3BO3 2.189e-006 2.193e-006 -5.660 -5.659 0.001

H2BO3- 3.264e-008 2.960e-008 -7.486 -7.529 -0.043

Ba 7.722e-007

Ba+2 7.215e-007 4.918e-007 -6.142 -6.308 -0.166

BaSO4 3.086e-008 3.092e-008 -7.511 -7.510 0.001

BaHCO3+ 1.877e-008 1.702e-008 -7.726 -7.769 -0.043

BaCO3 1.094e-009 1.096e-009 -8.961 -8.960 0.001

BaOH+ 5.413e-013 4.908e-013 -12.267 -12.309 -0.043

C(4) 6.420e-003

HCO3- 5.792e-003 5.268e-003 -2.237 -2.278 -0.041

CO2 4.866e-004 4.877e-004 -3.313 -3.312 0.001

CaHCO3+ 8.671e-005 7.887e-005 -4.062 -4.103 -0.041

MgHCO3+ 3.227e-005 2.926e-005 -4.491 -4.534 -0.043

CaCO3 1.141e-005 1.143e-005 -4.943 -4.942 0.001

CO3-2 8.021e-006 5.489e-006 -5.096 -5.260 -0.165

MgCO3 2.143e-006 2.147e-006 -5.669 -5.668 0.001

NaHCO3 4.935e-007 4.945e-007 -6.307 -6.306 0.001

SrHCO3+ 3.655e-007 3.325e-007 -6.437 -6.478 -0.041

BaHCO3+ 1.877e-008 1.702e-008 -7.726 -7.769 -0.043

SrCO3 1.526e-008 1.530e-008 -7.816 -7.815 0.001

NaCO3- 1.002e-008 9.082e-009 -7.999 -8.042 -0.043

BaCO3 1.094e-009 1.096e-009 -8.961 -8.960 0.001

Ca 2.307e-003

Ca+2 2.175e-003 1.488e-003 -2.662 -2.827 -0.165

CaHCO3+ 8.671e-005 7.887e-005 -4.062 -4.103 -0.041

CaSO4 3.307e-005 3.314e-005 -4.481 -4.480 0.001

CaCO3 1.141e-005 1.143e-005 -4.943 -4.942 0.001

CaOH+ 8.023e-009 7.274e-009 -8.096 -8.138 -0.043

CaHSO4+ 6.373e-012 5.778e-012 -11.196 -11.238 -0.043

Cl 7.309e-005

Cl- 7.309e-005 6.616e-005 -4.136 -4.179 -0.043

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.435 -43.434 0.001

K 2.198e-005

K+ 2.196e-005 1.988e-005 -4.658 -4.702 -0.043

KSO4- 1.554e-008 1.409e-008 -7.808 -7.851 -0.043

KOH 2.026e-012 2.031e-012 -11.693 -11.692 0.001

Li 6.056e-006

Li+ 6.053e-006 5.513e-006 -5.218 -5.259 -0.041

LiSO4- 3.330e-009 3.020e-009 -8.477 -8.520 -0.043

LiOH 3.713e-012 3.721e-012 -11.430 -11.429 0.001

Mg 7.613e-004

Mg+2 7.164e-004 4.929e-004 -3.145 -3.307 -0.162

MgHCO3+ 3.227e-005 2.926e-005 -4.491 -4.534 -0.043

MgSO4 1.048e-005 1.051e-005 -4.979 -4.979 0.001

MgCO3 2.143e-006 2.147e-006 -5.669 -5.668 0.001

MgOH+ 1.880e-008 1.705e-008 -7.726 -7.768 -0.043

N(5) 4.857e-006

NO3- 4.857e-006 4.389e-006 -5.314 -5.358 -0.044

Na 1.845e-004

Na+ 1.839e-004 1.669e-004 -3.735 -3.777 -0.042

NaHCO3 4.935e-007 4.945e-007 -6.307 -6.306 0.001

NaSO4- 1.070e-007 9.697e-008 -6.971 -7.013 -0.043

NaCO3- 1.002e-008 9.082e-009 -7.999 -8.042 -0.043

NaOH 3.242e-011 3.249e-011 -10.489 -10.488 0.001

O(0) 5.672e-010

O2 2.836e-010 2.842e-010 -9.547 -9.546 0.001

S(6) 2.281e-004

SO4-2 1.842e-004 1.255e-004 -3.735 -3.901 -0.167

CaSO4 3.307e-005 3.314e-005 -4.481 -4.480 0.001

MgSO4 1.048e-005 1.051e-005 -4.979 -4.979 0.001

SrSO4 1.311e-007 1.314e-007 -6.882 -6.881 0.001

NaSO4- 1.070e-007 9.697e-008 -6.971 -7.013 -0.043

BaSO4 3.086e-008 3.092e-008 -7.511 -7.510 0.001

KSO4- 1.554e-008 1.409e-008 -7.808 -7.851 -0.043

LiSO4- 3.330e-009 3.020e-009 -8.477 -8.520 -0.043

HSO4- 3.562e-010 3.230e-010 -9.448 -9.491 -0.043

CaHSO4+ 6.373e-012 5.778e-012 -11.196 -11.238 -0.043

AlSO4+ 3.015e-012 2.734e-012 -11.521 -11.563 -0.043

Al(SO4)2- 1.129e-014 1.024e-014 -13.947 -13.990 -0.043

AlHSO4+2 1.117e-020 7.548e-021 -19.952 -20.122 -0.170

Si 9.825e-005

H4SiO4 9.795e-005 9.816e-005 -4.009 -4.008 0.001

H3SiO4- 2.993e-007 2.713e-007 -6.524 -6.566 -0.043

H2SiO4-2 3.475e-013 2.349e-013 -12.459 -12.629 -0.170

Sr 9.592e-006

Sr+2 9.080e-006 6.222e-006 -5.042 -5.206 -0.164

SrHCO3+ 3.655e-007 3.325e-007 -6.437 -6.478 -0.041

SrSO4 1.311e-007 1.314e-007 -6.882 -6.881 0.001

SrCO3 1.526e-008 1.530e-008 -7.816 -7.815 0.001

SrOH+ 1.034e-011 9.399e-012 -10.985 -11.027 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -0.30 11.32 11.61 Al(OH)3

Albite -2.19 -20.99 -18.80 NaAlSi3O8

Alunite -1.11 -0.96 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.39 -6.73 -4.33 CaSO4

Anorthite -1.14 -21.21 -20.07 CaAl2Si2O8

Aragonite 0.18 -8.09 -8.27 CaCO3

Barite -0.03 -10.21 -10.18 BaSO4

Ca-Montmorillonite 4.63 -42.20 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.33 -8.09 -8.42 CaCO3

Celestite -2.48 -9.11 -6.62 SrSO4

Chalcedony -0.31 -4.01 -3.70 SiO2

Chlorite(14A) -4.27 68.76 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -6.87 26.88 33.75 Mg3Si2O5(OH)4

CO2(g) -2.00 -3.31 -1.31 CO2

Dolomite 0.14 -16.66 -16.80 CaMg(CO3)2

Gibbsite 2.51 11.32 8.81 Al(OH)3

Gypsum -2.14 -6.73 -4.59 CaSO4:2H2O

H2(g) -40.34 -43.43 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.51 -7.96 1.55 NaCl

Illite 3.38 -38.57 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -0.39 -21.91 -21.52 KAlSi3O8

K-mica 10.16 24.69 14.53 KAl3Si3O10(OH)2

Kaolinite 6.10 14.62 8.52 Al2Si2O5(OH)4

O2(g) -6.75 -9.55 -2.79 O2

Quartz 0.16 -4.01 -4.16 SiO2

Sepiolite -4.85 11.24 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -7.42 11.24 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.19 -4.01 -2.81 SiO2

Strontianite -1.19 -10.47 -9.28 SrCO3

Talc -3.96 18.86 22.82 Mg3Si4O10(OH)2

Witherite -2.96 -11.57 -8.61 BaCO3

Initial solution 8. 09-1-6

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 8.232e-006 8.232e-006

Alkalinity 5.854e-003 5.854e-003

B 1.573e-006 1.573e-006

Ba 7.139e-007 7.139e-007

Ca 2.217e-003 2.217e-003

Cl 6.096e-005 6.096e-005

K 9.135e-006 9.135e-006

Li 1.442e-006 1.442e-006

Mg 7.490e-004 7.490e-004

N(5) 2.214e-006 2.214e-006

Na 1.854e-004 1.854e-004

S(6) 2.791e-004 2.791e-004

Si 8.592e-005 8.592e-005

Sr 9.249e-006 9.249e-006

----------------------------Description of solution----------------------------

pH = 7.802 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 416

Density (g/cm3) = 0.99979

Activity of water = 1.000

Ionic strength = 9.056e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 5.996e-003

Total CO2 (mol/kg) = 5.996e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -3.031e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -2.51

Iterations = 11

Total H = 1.110185e+002

Total O = 5.552549e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.659e-007 2.409e-007 -6.575 -6.618 -0.043

H+ 1.719e-008 1.578e-008 -7.765 -7.802 -0.037

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 8.232e-006

Al(OH)4- 8.141e-006 7.389e-006 -5.089 -5.131 -0.042

Al(OH)3 6.964e-008 6.979e-008 -7.157 -7.156 0.001

Al(OH)2+ 2.149e-008 1.951e-008 -7.668 -7.710 -0.042

AlOH+2 1.785e-010 1.212e-010 -9.748 -9.917 -0.168

Al+3 9.268e-013 4.291e-013 -12.033 -12.367 -0.334

AlSO4+ 1.973e-013 1.790e-013 -12.705 -12.747 -0.042

Al(SO4)2- 9.133e-016 8.290e-016 -15.039 -15.081 -0.042

AlHSO4+2 3.386e-022 2.299e-022 -21.470 -21.639 -0.168

B 1.573e-006

H3BO3 1.525e-006 1.528e-006 -5.817 -5.816 0.001

H2BO3- 4.884e-008 4.434e-008 -7.311 -7.353 -0.042

Ba 7.139e-007

Ba+2 6.600e-007 4.518e-007 -6.180 -6.345 -0.165

BaSO4 3.506e-008 3.513e-008 -7.455 -7.454 0.001

BaHCO3+ 1.673e-008 1.519e-008 -7.776 -7.818 -0.042

BaCO3 2.099e-009 2.103e-009 -8.678 -8.677 0.001

BaOH+ 1.068e-012 9.698e-013 -11.971 -12.013 -0.042

C(4) 5.996e-003

HCO3- 5.620e-003 5.117e-003 -2.250 -2.291 -0.041

CO2 2.198e-004 2.203e-004 -3.658 -3.657 0.001

CaHCO3+ 8.055e-005 7.334e-005 -4.094 -4.135 -0.041

MgHCO3+ 3.076e-005 2.792e-005 -4.512 -4.554 -0.042

CaCO3 2.282e-005 2.287e-005 -4.642 -4.641 0.001

CO3-2 1.668e-005 1.147e-005 -4.778 -4.941 -0.163

MgCO3 4.398e-006 4.407e-006 -5.357 -5.356 0.001

NaHCO3 4.820e-007 4.830e-007 -6.317 -6.316 0.001

SrHCO3+ 3.420e-007 3.114e-007 -6.466 -6.507 -0.041

SrCO3 3.075e-008 3.081e-008 -7.512 -7.511 0.001

NaCO3- 2.102e-008 1.908e-008 -7.677 -7.719 -0.042

BaHCO3+ 1.673e-008 1.519e-008 -7.776 -7.818 -0.042

BaCO3 2.099e-009 2.103e-009 -8.678 -8.677 0.001

Ca 2.217e-003

Ca+2 2.074e-003 1.425e-003 -2.683 -2.846 -0.163

CaHCO3+ 8.055e-005 7.334e-005 -4.094 -4.135 -0.041

CaSO4 3.916e-005 3.925e-005 -4.407 -4.406 0.001

CaCO3 2.282e-005 2.287e-005 -4.642 -4.641 0.001

CaOH+ 1.650e-008 1.498e-008 -7.783 -7.825 -0.042

CaHSO4+ 3.505e-012 3.182e-012 -11.455 -11.497 -0.042

Cl 6.096e-005

Cl- 6.096e-005 5.524e-005 -4.215 -4.258 -0.043

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -44.100 -44.100 0.001

K 9.135e-006

K+ 9.127e-006 8.271e-006 -5.040 -5.082 -0.043

KSO4- 7.988e-009 7.250e-009 -8.098 -8.140 -0.042

KOH 1.813e-012 1.817e-012 -11.742 -11.741 0.001

Li 1.442e-006

Li+ 1.441e-006 1.314e-006 -5.841 -5.881 -0.040

LiSO4- 9.804e-010 8.899e-010 -9.009 -9.051 -0.042

LiOH 1.903e-012 1.907e-012 -11.721 -11.720 0.001

Mg 7.490e-004

Mg+2 7.010e-004 4.843e-004 -3.154 -3.315 -0.161

MgHCO3+ 3.076e-005 2.792e-005 -4.512 -4.554 -0.042

MgSO4 1.274e-005 1.277e-005 -4.895 -4.894 0.001

MgCO3 4.398e-006 4.407e-006 -5.357 -5.356 0.001

MgOH+ 3.968e-008 3.602e-008 -7.401 -7.443 -0.042

N(5) 2.214e-006

NO3- 2.214e-006 2.003e-006 -5.655 -5.698 -0.043

Na 1.854e-004

Na+ 1.848e-004 1.679e-004 -3.733 -3.775 -0.042

NaHCO3 4.820e-007 4.830e-007 -6.317 -6.316 0.001

NaSO4- 1.329e-007 1.206e-007 -6.877 -6.919 -0.042

NaCO3- 2.102e-008 1.908e-008 -7.677 -7.719 -0.042

NaOH 7.012e-011 7.026e-011 -10.154 -10.153 0.001

O(0) 1.213e-008

O2 6.067e-009 6.079e-009 -8.217 -8.216 0.001

S(6) 2.791e-004

SO4-2 2.269e-004 1.552e-004 -3.644 -3.809 -0.165

CaSO4 3.916e-005 3.925e-005 -4.407 -4.406 0.001

MgSO4 1.274e-005 1.277e-005 -4.895 -4.894 0.001

SrSO4 1.563e-007 1.567e-007 -6.806 -6.805 0.001

NaSO4- 1.329e-007 1.206e-007 -6.877 -6.919 -0.042

BaSO4 3.506e-008 3.513e-008 -7.455 -7.454 0.001

KSO4- 7.988e-009 7.250e-009 -8.098 -8.140 -0.042

LiSO4- 9.804e-010 8.899e-010 -9.009 -9.051 -0.042

HSO4- 2.046e-010 1.858e-010 -9.689 -9.731 -0.042

CaHSO4+ 3.505e-012 3.182e-012 -11.455 -11.497 -0.042

AlSO4+ 1.973e-013 1.790e-013 -12.705 -12.747 -0.042

Al(SO4)2- 9.133e-016 8.290e-016 -15.039 -15.081 -0.042

AlHSO4+2 3.386e-022 2.299e-022 -21.470 -21.639 -0.168

Si 8.592e-005

H4SiO4 8.536e-005 8.554e-005 -4.069 -4.068 0.001

H3SiO4- 5.602e-007 5.085e-007 -6.252 -6.294 -0.042

H2SiO4-2 1.394e-012 9.465e-013 -11.856 -12.024 -0.168

Sr 9.249e-006

Sr+2 8.720e-006 6.000e-006 -5.059 -5.222 -0.162

SrHCO3+ 3.420e-007 3.114e-007 -6.466 -6.507 -0.041

SrSO4 1.563e-007 1.567e-007 -6.806 -6.805 0.001

SrCO3 3.075e-008 3.081e-008 -7.512 -7.511 0.001

SrOH+ 2.143e-011 1.949e-011 -10.669 -10.710 -0.041

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -0.58 11.04 11.61 Al(OH)3

Albite -2.31 -21.11 -18.80 NaAlSi3O8

Alunite -3.14 -2.99 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.32 -6.66 -4.33 CaSO4

Anorthite -1.17 -21.24 -20.07 CaAl2Si2O8

Aragonite 0.48 -7.79 -8.27 CaCO3

Barite 0.03 -10.15 -10.18 BaSO4

Ca-Montmorillonite 3.86 -42.96 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.63 -7.79 -8.42 CaCO3

Celestite -2.41 -9.03 -6.62 SrSO4

Chalcedony -0.37 -4.07 -3.70 SiO2

Chlorite(14A) -1.72 71.32 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -5.02 28.73 33.75 Mg3Si2O5(OH)4

CO2(g) -2.34 -3.66 -1.31 CO2

Dolomite 0.76 -16.04 -16.80 CaMg(CO3)2

Gibbsite 2.23 11.04 8.81 Al(OH)3

Gypsum -2.07 -6.66 -4.59 CaSO4:2H2O

H2(g) -41.00 -44.10 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.59 -8.03 1.55 NaCl

Illite 2.67 -39.28 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -0.90 -22.42 -21.52 KAlSi3O8

K-mica 9.10 23.63 14.53 KAl3Si3O10(OH)2

Kaolinite 5.42 13.94 8.52 Al2Si2O5(OH)4

O2(g) -5.42 -8.22 -2.79 O2

Quartz 0.10 -4.07 -4.16 SiO2

Sepiolite -3.71 12.37 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -6.29 12.37 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.25 -4.07 -2.81 SiO2

Strontianite -0.88 -10.16 -9.28 SrCO3

Talc -2.23 20.60 22.82 Mg3Si4O10(OH)2

Witherite -2.68 -11.29 -8.61 BaCO3

Initial solution 9. 09-2-21

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 4.746e-006 4.746e-006

Alkalinity 5.788e-003 5.788e-003

B 1.481e-006 1.481e-006

Ba 6.921e-007 6.921e-007

Ca 2.304e-003 2.304e-003

Cl 6.350e-005 6.350e-005

K 1.085e-005 1.085e-005

Li 5.335e-006 5.335e-006

Mg 7.696e-004 7.696e-004

N(5) 4.429e-006 4.429e-006

Na 1.854e-004 1.854e-004

S(6) 3.479e-004 3.479e-004

Si 8.126e-005 8.126e-005

Sr 9.363e-006 9.363e-006

----------------------------Description of solution----------------------------

pH = 7.974 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 425

Density (g/cm3) = 0.99980

Activity of water = 1.000

Ionic strength = 9.297e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 5.848e-003

Total CO2 (mol/kg) = 5.848e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -1.685e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.38

Iterations = 11

Total H = 1.110184e+002

Total O = 5.552537e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.959e-007 3.583e-007 -6.402 -6.446 -0.043

H+ 1.157e-008 1.061e-008 -7.937 -7.974 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 4.746e-006

Al(OH)4- 4.714e-006 4.274e-006 -5.327 -5.369 -0.043

Al(OH)3 2.708e-008 2.714e-008 -7.567 -7.566 0.001

Al(OH)2+ 5.625e-009 5.100e-009 -8.250 -8.292 -0.043

AlOH+2 3.152e-011 2.130e-011 -10.501 -10.672 -0.170

Al+3 1.104e-013 5.071e-014 -12.957 -13.295 -0.338

AlSO4+ 2.885e-014 2.616e-014 -13.540 -13.582 -0.043

Al(SO4)2- 1.652e-016 1.497e-016 -15.782 -15.825 -0.043

AlHSO4+2 3.341e-023 2.258e-023 -22.476 -22.646 -0.170

B 1.481e-006

H3BO3 1.413e-006 1.416e-006 -5.850 -5.849 0.001

H2BO3- 6.743e-008 6.114e-008 -7.171 -7.214 -0.043

Ba 6.921e-007

Ba+2 6.321e-007 4.308e-007 -6.199 -6.366 -0.167

BaSO4 4.133e-008 4.142e-008 -7.384 -7.383 0.001

BaHCO3+ 1.569e-008 1.422e-008 -7.804 -7.847 -0.043

BaCO3 2.923e-009 2.929e-009 -8.534 -8.533 0.001

BaOH+ 1.517e-012 1.375e-012 -11.819 -11.862 -0.043

C(4) 5.848e-003

HCO3- 5.524e-003 5.025e-003 -2.258 -2.299 -0.041

CO2 1.451e-004 1.454e-004 -3.838 -3.837 0.001

CaHCO3+ 8.130e-005 7.395e-005 -4.090 -4.131 -0.041

CaCO3 3.422e-005 3.429e-005 -4.466 -4.465 0.001

MgHCO3+ 3.077e-005 2.789e-005 -4.512 -4.554 -0.043

CO3-2 2.447e-005 1.675e-005 -4.611 -4.776 -0.165

MgCO3 6.535e-006 6.549e-006 -5.185 -5.184 0.001

NaHCO3 4.727e-007 4.737e-007 -6.325 -6.324 0.001

SrHCO3+ 3.374e-007 3.068e-007 -6.472 -6.513 -0.041

SrCO3 4.506e-008 4.515e-008 -7.346 -7.345 0.001

NaCO3- 3.069e-008 2.783e-008 -7.513 -7.556 -0.043

BaHCO3+ 1.569e-008 1.422e-008 -7.804 -7.847 -0.043

BaCO3 2.923e-009 2.929e-009 -8.534 -8.533 0.001

Ca 2.304e-003

Ca+2 2.139e-003 1.463e-003 -2.670 -2.835 -0.165

CaHCO3+ 8.130e-005 7.395e-005 -4.090 -4.131 -0.041

CaSO4 4.971e-005 4.982e-005 -4.304 -4.303 0.001

CaCO3 3.422e-005 3.429e-005 -4.466 -4.465 0.001

CaOH+ 2.523e-008 2.287e-008 -7.598 -7.641 -0.043

CaHSO4+ 2.995e-012 2.715e-012 -11.524 -11.566 -0.043

Cl 6.350e-005

Cl- 6.350e-005 5.748e-005 -4.197 -4.241 -0.043

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -44.445 -44.444 0.001

K 1.085e-005

K+ 1.084e-005 9.810e-006 -4.965 -5.008 -0.043

KSO4- 1.173e-008 1.063e-008 -7.931 -7.973 -0.043

KOH 3.198e-012 3.205e-012 -11.495 -11.494 0.001

Li 5.335e-006

Li+ 5.330e-006 4.856e-006 -5.273 -5.314 -0.041

LiSO4- 4.484e-009 4.066e-009 -8.348 -8.391 -0.043

LiOH 1.046e-011 1.048e-011 -10.981 -10.980 0.001

Mg 7.696e-004

Mg+2 7.162e-004 4.927e-004 -3.145 -3.307 -0.162

MgHCO3+ 3.077e-005 2.789e-005 -4.512 -4.554 -0.043

MgSO4 1.602e-005 1.606e-005 -4.795 -4.794 0.001

MgCO3 6.535e-006 6.549e-006 -5.185 -5.184 0.001

MgOH+ 6.011e-008 5.450e-008 -7.221 -7.264 -0.043

N(5) 4.429e-006

NO3- 4.429e-006 4.002e-006 -5.354 -5.398 -0.044

Na 1.854e-004

Na+ 1.847e-004 1.677e-004 -3.733 -3.776 -0.042

NaHCO3 4.727e-007 4.737e-007 -6.325 -6.324 0.001

NaSO4- 1.642e-007 1.489e-007 -6.785 -6.827 -0.043

NaCO3- 3.069e-008 2.783e-008 -7.513 -7.556 -0.043

NaOH 1.041e-010 1.044e-010 -9.982 -9.981 0.001

O(0) 5.938e-008

O2 2.969e-008 2.975e-008 -7.527 -7.526 0.001

S(6) 3.479e-004

SO4-2 2.817e-004 1.918e-004 -3.550 -3.717 -0.167

CaSO4 4.971e-005 4.982e-005 -4.304 -4.303 0.001

MgSO4 1.602e-005 1.606e-005 -4.795 -4.794 0.001

SrSO4 1.939e-007 1.944e-007 -6.712 -6.711 0.001

NaSO4- 1.642e-007 1.489e-007 -6.785 -6.827 -0.043

BaSO4 4.133e-008 4.142e-008 -7.384 -7.383 0.001

KSO4- 1.173e-008 1.063e-008 -7.931 -7.973 -0.043

LiSO4- 4.484e-009 4.066e-009 -8.348 -8.391 -0.043

HSO4- 1.703e-010 1.544e-010 -9.769 -9.811 -0.043

CaHSO4+ 2.995e-012 2.715e-012 -11.524 -11.566 -0.043

AlSO4+ 2.885e-014 2.616e-014 -13.540 -13.582 -0.043

Al(SO4)2- 1.652e-016 1.497e-016 -15.782 -15.825 -0.043

AlHSO4+2 3.341e-023 2.258e-023 -22.476 -22.646 -0.170

Si 8.126e-005

H4SiO4 8.047e-005 8.065e-005 -4.094 -4.093 0.001

H3SiO4- 7.865e-007 7.131e-007 -6.104 -6.147 -0.043

H2SiO4-2 2.921e-012 1.974e-012 -11.534 -11.705 -0.170

Sr 9.363e-006

Sr+2 8.787e-006 6.020e-006 -5.056 -5.220 -0.164

SrHCO3+ 3.374e-007 3.068e-007 -6.472 -6.513 -0.041

SrSO4 1.939e-007 1.944e-007 -6.712 -6.711 0.001

SrCO3 4.506e-008 4.515e-008 -7.346 -7.345 0.001

SrOH+ 3.202e-011 2.909e-011 -10.495 -10.536 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -0.99 10.63 11.61 Al(OH)3

Albite -2.63 -21.42 -18.80 NaAlSi3O8

Alunite -4.63 -4.48 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.22 -6.55 -4.33 CaSO4

Anorthite -1.69 -21.76 -20.07 CaAl2Si2O8

Aragonite 0.66 -7.61 -8.27 CaCO3

Barite 0.10 -10.08 -10.18 BaSO4

Ca-Montmorillonite 2.87 -43.95 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.81 -7.61 -8.42 CaCO3

Celestite -2.31 -8.94 -6.62 SrSO4

Chalcedony -0.40 -4.09 -3.70 SiO2

Chlorite(14A) -0.86 72.18 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -4.01 29.74 33.75 Mg3Si2O5(OH)4

CO2(g) -2.52 -3.84 -1.31 CO2

Dolomite 1.11 -15.69 -16.80 CaMg(CO3)2

Gibbsite 1.82 10.63 8.81 Al(OH)3

Gypsum -1.97 -6.55 -4.59 CaSO4:2H2O

H2(g) -41.35 -44.44 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.57 -8.02 1.55 NaCl

Illite 1.87 -40.08 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -1.14 -22.66 -21.52 KAlSi3O8

K-mica 8.04 22.57 14.53 KAl3Si3O10(OH)2

Kaolinite 4.55 13.07 8.52 Al2Si2O5(OH)4

O2(g) -4.73 -7.53 -2.79 O2

Quartz 0.07 -4.09 -4.16 SiO2

Sepiolite -3.09 13.00 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -5.66 13.00 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.28 -4.09 -2.81 SiO2

Strontianite -0.72 -10.00 -9.28 SrCO3

Talc -1.27 21.55 22.82 Mg3Si4O10(OH)2

Witherite -2.53 -11.14 -8.61 BaCO3

Initial solution 10. 09-4-18

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 1.698e-005 1.698e-005

Alkalinity 5.952e-003 5.952e-003

B 1.759e-006 1.759e-006

Ba 7.285e-007 7.285e-007

Ca 2.269e-003 2.269e-003

Cl 6.039e-005 6.039e-005

K 1.221e-005 1.221e-005

Li 5.191e-006 5.191e-006

Mg 7.531e-004 7.531e-004

Na 1.897e-004 1.897e-004

S(6) 1.687e-004 1.687e-004

Si 1.004e-004 1.004e-004

Sr 8.907e-006 8.907e-006

----------------------------Description of solution----------------------------

pH = 7.899 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 414

Density (g/cm3) = 0.99979

Activity of water = 1.000

Ionic strength = 9.042e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.004e-003

Total CO2 (mol/kg) = 6.004e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -2.803e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.23

Iterations = 11

Total H = 1.110187e+002

Total O = 5.552520e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.326e-007 3.013e-007 -6.478 -6.521 -0.043

H+ 1.374e-008 1.262e-008 -7.862 -7.899 -0.037

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 1.698e-005

Al(OH)4- 1.684e-005 1.529e-005 -4.774 -4.816 -0.042

Al(OH)3 1.152e-007 1.154e-007 -6.939 -6.938 0.001

Al(OH)2+ 2.841e-008 2.579e-008 -7.546 -7.589 -0.042

AlOH+2 1.887e-010 1.281e-010 -9.724 -9.892 -0.168

Al+3 7.828e-013 3.626e-013 -12.106 -12.441 -0.334

AlSO4+ 1.003e-013 9.107e-014 -12.999 -13.041 -0.042

Al(SO4)2- 2.796e-016 2.538e-016 -15.553 -15.595 -0.042

AlHSO4+2 1.377e-022 9.348e-023 -21.861 -22.029 -0.168

B 1.759e-006

H3BO3 1.691e-006 1.694e-006 -5.772 -5.771 0.001

H2BO3- 6.775e-008 6.150e-008 -7.169 -7.211 -0.042

Ba 7.285e-007

Ba+2 6.863e-007 4.699e-007 -6.164 -6.328 -0.165

BaSO4 2.195e-008 2.200e-008 -7.659 -7.658 0.001

BaHCO3+ 1.751e-008 1.590e-008 -7.757 -7.799 -0.042

BaCO3 2.748e-009 2.753e-009 -8.561 -8.560 0.001

BaOH+ 1.390e-012 1.262e-012 -11.857 -11.899 -0.042

C(4) 6.004e-003

HCO3- 5.655e-003 5.149e-003 -2.248 -2.288 -0.041

CO2 1.768e-004 1.772e-004 -3.752 -3.752 0.001

CaHCO3+ 8.334e-005 7.588e-005 -4.079 -4.120 -0.041

MgHCO3+ 3.129e-005 2.840e-005 -4.505 -4.547 -0.042

CaCO3 2.953e-005 2.959e-005 -4.530 -4.529 0.001

CO3-2 2.100e-005 1.443e-005 -4.678 -4.841 -0.163

MgCO3 5.595e-006 5.607e-006 -5.252 -5.251 0.001

NaHCO3 4.966e-007 4.977e-007 -6.304 -6.303 0.001

SrHCO3+ 3.334e-007 3.035e-007 -6.477 -6.518 -0.041

SrCO3 3.749e-008 3.757e-008 -7.426 -7.425 0.001

NaCO3- 2.708e-008 2.459e-008 -7.567 -7.609 -0.042

BaHCO3+ 1.751e-008 1.590e-008 -7.757 -7.799 -0.042

BaCO3 2.748e-009 2.753e-009 -8.561 -8.560 0.001

Ca 2.269e-003

Ca+2 2.132e-003 1.465e-003 -2.671 -2.834 -0.163

CaHCO3+ 8.334e-005 7.588e-005 -4.079 -4.120 -0.041

CaCO3 2.953e-005 2.959e-005 -4.530 -4.529 0.001

CaSO4 2.424e-005 2.429e-005 -4.616 -4.615 0.001

CaOH+ 2.122e-008 1.926e-008 -7.673 -7.715 -0.042

CaHSO4+ 1.734e-012 1.574e-012 -11.761 -11.803 -0.042

Cl 6.039e-005

Cl- 6.039e-005 5.473e-005 -4.219 -4.262 -0.043

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -44.295 -44.294 0.001

K 1.221e-005

K+ 1.220e-005 1.106e-005 -4.914 -4.956 -0.043

KSO4- 6.426e-009 5.833e-009 -8.192 -8.234 -0.042

KOH 3.031e-012 3.038e-012 -11.518 -11.517 0.001

Li 5.191e-006

Li+ 5.189e-006 4.731e-006 -5.285 -5.325 -0.040

LiSO4- 2.125e-009 1.929e-009 -8.673 -8.715 -0.042

LiOH 8.571e-012 8.589e-012 -11.067 -11.066 0.001

Mg 7.531e-004

Mg+2 7.084e-004 4.895e-004 -3.150 -3.310 -0.161

MgHCO3+ 3.129e-005 2.840e-005 -4.505 -4.547 -0.042

MgSO4 7.751e-006 7.767e-006 -5.111 -5.110 0.001

MgCO3 5.595e-006 5.607e-006 -5.252 -5.251 0.001

MgOH+ 5.016e-008 4.554e-008 -7.300 -7.342 -0.042

Na 1.897e-004

Na+ 1.891e-004 1.719e-004 -3.723 -3.765 -0.042

NaHCO3 4.966e-007 4.977e-007 -6.304 -6.303 0.001

NaSO4- 8.187e-008 7.432e-008 -7.087 -7.129 -0.042

NaCO3- 2.708e-008 2.459e-008 -7.567 -7.609 -0.042

NaOH 8.979e-011 8.998e-011 -10.047 -10.046 0.001

O(0) 2.970e-008

O2 1.485e-008 1.488e-008 -7.828 -7.827 0.001

S(6) 1.687e-004

SO4-2 1.365e-004 9.340e-005 -3.865 -4.030 -0.165

CaSO4 2.424e-005 2.429e-005 -4.616 -4.615 0.001

MgSO4 7.751e-006 7.767e-006 -5.111 -5.110 0.001

SrSO4 9.116e-008 9.135e-008 -7.040 -7.039 0.001

NaSO4- 8.187e-008 7.432e-008 -7.087 -7.129 -0.042

BaSO4 2.195e-008 2.200e-008 -7.659 -7.658 0.001

KSO4- 6.426e-009 5.833e-009 -8.192 -8.234 -0.042

LiSO4- 2.125e-009 1.929e-009 -8.673 -8.715 -0.042

HSO4- 9.847e-011 8.939e-011 -10.007 -10.049 -0.042

CaHSO4+ 1.734e-012 1.574e-012 -11.761 -11.803 -0.042

AlSO4+ 1.003e-013 9.107e-014 -12.999 -13.041 -0.042

Al(SO4)2- 2.796e-016 2.538e-016 -15.553 -15.595 -0.042

AlHSO4+2 1.377e-022 9.348e-023 -21.861 -22.029 -0.168

Si 1.004e-004

H4SiO4 9.959e-005 9.980e-005 -4.002 -4.001 0.001

H3SiO4- 8.175e-007 7.421e-007 -6.088 -6.130 -0.042

H2SiO4-2 2.545e-012 1.728e-012 -11.594 -11.762 -0.168

Sr 8.907e-006

Sr+2 8.445e-006 5.812e-006 -5.073 -5.236 -0.162

SrHCO3+ 3.334e-007 3.035e-007 -6.477 -6.518 -0.041

SrSO4 9.116e-008 9.135e-008 -7.040 -7.039 0.001

SrCO3 3.749e-008 3.757e-008 -7.426 -7.425 0.001

SrOH+ 2.596e-011 2.362e-011 -10.586 -10.627 -0.041

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -0.36 11.26 11.61 Al(OH)3

Albite -1.78 -20.58 -18.80 NaAlSi3O8

Alunite -3.09 -2.94 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.53 -6.86 -4.33 CaSO4

Anorthite -0.40 -20.47 -20.07 CaAl2Si2O8

Aragonite 0.59 -7.67 -8.27 CaCO3

Barite -0.17 -10.36 -10.18 BaSO4

Ca-Montmorillonite 4.65 -42.17 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.75 -7.67 -8.42 CaCO3

Celestite -2.64 -9.27 -6.62 SrSO4

Chalcedony -0.30 -4.00 -3.70 SiO2

Chlorite(14A) -0.09 72.95 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -4.29 29.46 33.75 Mg3Si2O5(OH)4

CO2(g) -2.44 -3.75 -1.31 CO2

Dolomite 0.97 -15.83 -16.80 CaMg(CO3)2

Gibbsite 2.45 11.26 8.81 Al(OH)3

Gypsum -2.28 -6.86 -4.59 CaSO4:2H2O

H2(g) -41.20 -44.29 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.58 -8.03 1.55 NaCl

Illite 3.59 -38.36 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -0.25 -21.77 -21.52 KAlSi3O8

K-mica 10.18 24.71 14.53 KAl3Si3O10(OH)2

Kaolinite 5.99 14.51 8.52 Al2Si2O5(OH)4

O2(g) -5.03 -7.83 -2.79 O2

Quartz 0.16 -4.00 -4.16 SiO2

Sepiolite -3.12 12.97 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -5.69 12.97 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.19 -4.00 -2.81 SiO2

Strontianite -0.80 -10.08 -9.28 SrCO3

Talc -1.36 21.46 22.82 Mg3Si4O10(OH)2

Witherite -2.56 -11.17 -8.61 BaCO3

Initial solution 11. 09-5-20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 2.967e-007 2.967e-007

Alkalinity 6.165e-003 6.165e-003

B 2.314e-006 2.314e-006

Ba 7.576e-007 7.576e-007

Ca 2.371e-003 2.371e-003

Cl 5.023e-005 5.023e-005

K 1.231e-005 1.231e-005

Li 5.047e-006 5.047e-006

Mg 7.572e-004 7.572e-004

N(5) 3.714e-006 3.714e-006

Na 1.945e-004 1.945e-004

S(6) 1.614e-004 1.614e-004

Si 9.242e-005 9.242e-005

Sr 9.363e-006 9.363e-006

----------------------------Description of solution----------------------------

pH = 7.740 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 429

Density (g/cm3) = 0.99981

Activity of water = 1.000

Ionic strength = 9.376e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.390e-003

Total CO2 (mol/kg) = 6.390e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -5.158e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.41

Iterations = 11

Total H = 1.110189e+002

Total O = 5.552615e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.307e-007 2.087e-007 -6.637 -6.680 -0.044

H+ 1.987e-008 1.822e-008 -7.702 -7.740 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 2.967e-007

Al(OH)4- 2.927e-007 2.653e-007 -6.534 -6.576 -0.043

Al(OH)3 2.886e-009 2.892e-009 -8.540 -8.539 0.001

Al(OH)2+ 1.029e-009 9.330e-010 -8.987 -9.030 -0.043

AlOH+2 9.913e-012 6.689e-012 -11.004 -11.175 -0.171

Al+3 5.967e-014 2.734e-014 -13.224 -13.563 -0.339

AlSO4+ 7.170e-015 6.498e-015 -14.144 -14.187 -0.043

Al(SO4)2- 1.891e-017 1.714e-017 -16.723 -16.766 -0.043

AlHSO4+2 1.427e-023 9.629e-024 -22.846 -23.016 -0.171

B 2.314e-006

H3BO3 2.251e-006 2.256e-006 -5.648 -5.647 0.001

H2BO3- 6.259e-008 5.673e-008 -7.203 -7.246 -0.043

Ba 7.576e-007

Ba+2 7.150e-007 4.866e-007 -6.146 -6.313 -0.167

BaSO4 2.151e-008 2.156e-008 -7.667 -7.666 0.001

BaHCO3+ 1.910e-008 1.731e-008 -7.719 -7.762 -0.043

BaCO3 2.072e-009 2.076e-009 -8.684 -8.683 0.001

BaOH+ 9.985e-013 9.050e-013 -12.001 -12.043 -0.043

C(4) 6.390e-003

HCO3- 5.954e-003 5.414e-003 -2.225 -2.267 -0.041

CO2 2.684e-004 2.689e-004 -3.571 -3.570 0.001

CaHCO3+ 9.140e-005 8.310e-005 -4.039 -4.080 -0.041

MgHCO3+ 3.296e-005 2.987e-005 -4.482 -4.525 -0.043

CaCO3 2.240e-005 2.245e-005 -4.650 -4.649 0.001

CO3-2 1.538e-005 1.051e-005 -4.813 -4.978 -0.165

MgCO3 4.077e-006 4.086e-006 -5.390 -5.389 0.001

NaHCO3 5.344e-007 5.356e-007 -6.272 -6.271 0.001

SrHCO3+ 3.669e-007 3.336e-007 -6.435 -6.477 -0.041

SrCO3 2.853e-008 2.860e-008 -7.545 -7.544 0.001

NaCO3- 2.022e-008 1.833e-008 -7.694 -7.737 -0.043

BaHCO3+ 1.910e-008 1.731e-008 -7.719 -7.762 -0.043

BaCO3 2.072e-009 2.076e-009 -8.684 -8.683 0.001

Ca 2.371e-003

Ca+2 2.234e-003 1.526e-003 -2.651 -2.817 -0.166

CaHCO3+ 9.140e-005 8.310e-005 -4.039 -4.080 -0.041

CaSO4 2.389e-005 2.394e-005 -4.622 -4.621 0.001

CaCO3 2.240e-005 2.245e-005 -4.650 -4.649 0.001

CaOH+ 1.533e-008 1.390e-008 -7.814 -7.857 -0.043

CaHSO4+ 2.472e-012 2.240e-012 -11.607 -11.650 -0.043

Cl 5.023e-005

Cl- 5.023e-005 4.545e-005 -4.299 -4.342 -0.043

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.976 -43.975 0.001

K 1.231e-005

K+ 1.230e-005 1.113e-005 -4.910 -4.953 -0.043

KSO4- 6.133e-009 5.559e-009 -8.212 -8.255 -0.043

KOH 2.114e-012 2.118e-012 -11.675 -11.674 0.001

Li 5.047e-006

Li+ 5.045e-006 4.594e-006 -5.297 -5.338 -0.041

LiSO4- 1.956e-009 1.773e-009 -8.709 -8.751 -0.043

LiOH 5.764e-012 5.776e-012 -11.239 -11.238 0.001

Mg 7.572e-004

Mg+2 7.128e-004 4.898e-004 -3.147 -3.310 -0.163

MgHCO3+ 3.296e-005 2.987e-005 -4.482 -4.525 -0.043

MgSO4 7.339e-006 7.355e-006 -5.134 -5.133 0.001

MgCO3 4.077e-006 4.086e-006 -5.390 -5.389 0.001

MgOH+ 3.482e-008 3.156e-008 -7.458 -7.501 -0.043

N(5) 3.714e-006

NO3- 3.714e-006 3.355e-006 -5.430 -5.474 -0.044

Na 1.945e-004

Na+ 1.939e-004 1.759e-004 -3.712 -3.755 -0.042

NaHCO3 5.344e-007 5.356e-007 -6.272 -6.271 0.001

NaSO4- 7.945e-008 7.200e-008 -7.100 -7.143 -0.043

NaCO3- 2.022e-008 1.833e-008 -7.694 -7.737 -0.043

NaOH 6.366e-011 6.380e-011 -10.196 -10.195 0.001

O(0) 6.838e-009

O2 3.419e-009 3.426e-009 -8.466 -8.465 0.001

S(6) 1.614e-004

SO4-2 1.300e-004 8.840e-005 -3.886 -4.054 -0.167

CaSO4 2.389e-005 2.394e-005 -4.622 -4.621 0.001

MgSO4 7.339e-006 7.355e-006 -5.134 -5.133 0.001

SrSO4 9.017e-008 9.037e-008 -7.045 -7.044 0.001

NaSO4- 7.945e-008 7.200e-008 -7.100 -7.143 -0.043

BaSO4 2.151e-008 2.156e-008 -7.667 -7.666 0.001

KSO4- 6.133e-009 5.559e-009 -8.212 -8.255 -0.043

LiSO4- 1.956e-009 1.773e-009 -8.709 -8.751 -0.043

HSO4- 1.348e-010 1.221e-010 -9.870 -9.913 -0.043

CaHSO4+ 2.472e-012 2.240e-012 -11.607 -11.650 -0.043

AlSO4+ 7.170e-015 6.498e-015 -14.144 -14.187 -0.043

Al(SO4)2- 1.891e-017 1.714e-017 -16.723 -16.766 -0.043

AlHSO4+2 1.427e-023 9.629e-024 -22.846 -23.016 -0.171

Si 9.242e-005

H4SiO4 9.189e-005 9.209e-005 -4.037 -4.036 0.001

H3SiO4- 5.234e-007 4.744e-007 -6.281 -6.324 -0.043

H2SiO4-2 1.134e-012 7.651e-013 -11.945 -12.116 -0.171

Sr 9.363e-006

Sr+2 8.878e-006 6.074e-006 -5.052 -5.217 -0.165

SrHCO3+ 3.669e-007 3.336e-007 -6.435 -6.477 -0.041

SrSO4 9.017e-008 9.037e-008 -7.045 -7.044 0.001

SrCO3 2.853e-008 2.860e-008 -7.545 -7.544 0.001

SrOH+ 1.883e-011 1.710e-011 -10.725 -10.767 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -1.96 9.66 11.61 Al(OH)3

Albite -3.64 -22.44 -18.80 NaAlSi3O8

Alunite -7.46 -7.31 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.54 -6.87 -4.33 CaSO4

Anorthite -3.97 -24.04 -20.07 CaAl2Si2O8

Aragonite 0.47 -7.79 -8.27 CaCO3

Barite -0.18 -10.37 -10.18 BaSO4

Ca-Montmorillonite 0.74 -46.08 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.63 -7.79 -8.42 CaCO3

Celestite -2.65 -9.27 -6.62 SrSO4

Chalcedony -0.34 -4.04 -3.70 SiO2

Chlorite(14A) -4.99 68.05 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -5.31 28.44 33.75 Mg3Si2O5(OH)4

CO2(g) -2.26 -3.57 -1.31 CO2

Dolomite 0.72 -16.08 -16.80 CaMg(CO3)2

Gibbsite 0.84 9.66 8.81 Al(OH)3

Gypsum -2.28 -6.87 -4.59 CaSO4:2H2O

H2(g) -40.88 -43.98 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.65 -8.10 1.55 NaCl

Illite -0.39 -42.34 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -2.12 -23.64 -21.52 KAlSi3O8

K-mica 5.12 19.64 14.53 KAl3Si3O10(OH)2

Kaolinite 2.72 11.24 8.52 Al2Si2O5(OH)4

O2(g) -5.67 -8.47 -2.79 O2

Quartz 0.13 -4.04 -4.16 SiO2

Sepiolite -3.86 12.23 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -6.43 12.23 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.22 -4.04 -2.81 SiO2

Strontianite -0.92 -10.19 -9.28 SrCO3

Talc -2.46 20.36 22.82 Mg3Si4O10(OH)2

Witherite -2.68 -11.29 -8.61 BaCO3

Initial solution 12. 09-7-7

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 3.671e-006 3.671e-006

Alkalinity 6.592e-003 6.592e-003

B 2.869e-006 2.869e-006

Ba 8.597e-007 8.597e-007

Ca 2.489e-003 2.489e-003

Cl 4.826e-005 4.826e-005

K 1.395e-005 1.395e-005

Li 5.479e-006 5.479e-006

Mg 7.943e-004 7.943e-004

N(5) 3.072e-006 3.072e-006

Na 2.098e-004 2.098e-004

S(6) 1.739e-004 1.739e-004

Si 1.099e-004 1.099e-004

Sr 1.005e-005 1.005e-005

----------------------------Description of solution----------------------------

pH = 7.472 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 453

Density (g/cm3) = 0.99983

Activity of water = 1.000

Ionic strength = 9.910e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.084e-003

Total CO2 (mol/kg) = 7.084e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -1.626e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.22

Iterations = 11

Total H = 1.110194e+002

Total O = 5.552810e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.248e-007 1.126e-007 -6.904 -6.948 -0.045

H+ 3.689e-008 3.376e-008 -7.433 -7.472 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 3.671e-006

Al(OH)4- 3.562e-006 3.221e-006 -5.448 -5.492 -0.044

Al(OH)3 6.493e-008 6.508e-008 -7.188 -7.187 0.001

Al(OH)2+ 4.304e-008 3.892e-008 -7.366 -7.410 -0.044

AlOH+2 7.739e-010 5.172e-010 -9.111 -9.286 -0.175

Al+3 8.698e-012 3.918e-012 -11.061 -11.407 -0.346

AlSO4+ 1.093e-012 9.881e-013 -11.961 -12.005 -0.044

Al(SO4)2- 3.059e-015 2.766e-015 -14.514 -14.558 -0.044

AlHSO4+2 4.061e-021 2.714e-021 -20.391 -20.566 -0.175

B 2.869e-006

H3BO3 2.827e-006 2.833e-006 -5.549 -5.548 0.001

H2BO3- 4.251e-008 3.844e-008 -7.372 -7.415 -0.044

Ba 8.597e-007

Ba+2 8.097e-007 5.460e-007 -6.092 -6.263 -0.171

BaSO4 2.561e-008 2.567e-008 -7.592 -7.591 0.001

BaHCO3+ 2.299e-008 2.078e-008 -7.639 -7.682 -0.044

BaCO3 1.342e-009 1.345e-009 -8.872 -8.871 0.001

BaOH+ 6.059e-013 5.478e-013 -12.218 -12.261 -0.044

C(4) 7.084e-003

HCO3- 6.387e-003 5.794e-003 -2.195 -2.237 -0.042

CO2 5.323e-004 5.336e-004 -3.274 -3.273 0.001

CaHCO3+ 1.021e-004 9.260e-005 -3.991 -4.033 -0.042

MgHCO3+ 3.673e-005 3.321e-005 -4.435 -4.479 -0.044

CaCO3 1.346e-005 1.350e-005 -4.871 -4.870 0.001

CO3-2 8.962e-006 6.069e-006 -5.048 -5.217 -0.169

MgCO3 2.445e-006 2.451e-006 -5.612 -5.611 0.001

NaHCO3 6.151e-007 6.165e-007 -6.211 -6.210 0.001

SrHCO3+ 4.179e-007 3.791e-007 -6.379 -6.421 -0.042

BaHCO3+ 2.299e-008 2.078e-008 -7.639 -7.682 -0.044

SrCO3 1.749e-008 1.753e-008 -7.757 -7.756 0.001

NaCO3- 1.259e-008 1.138e-008 -7.900 -7.944 -0.044

BaCO3 1.342e-009 1.345e-009 -8.872 -8.871 0.001

Ca 2.489e-003

Ca+2 2.347e-003 1.588e-003 -2.629 -2.799 -0.170

CaHCO3+ 1.021e-004 9.260e-005 -3.991 -4.033 -0.042

CaSO4 2.639e-005 2.645e-005 -4.579 -4.578 0.001

CaCO3 1.346e-005 1.350e-005 -4.871 -4.870 0.001

CaOH+ 8.634e-009 7.806e-009 -8.064 -8.108 -0.044

CaHSO4+ 5.073e-012 4.587e-012 -11.295 -11.338 -0.044

Cl 4.826e-005

Cl- 4.826e-005 4.356e-005 -4.316 -4.361 -0.045

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.440 -43.439 0.001

K 1.395e-005

K+ 1.394e-005 1.258e-005 -4.856 -4.900 -0.045

KSO4- 7.373e-009 6.666e-009 -8.132 -8.176 -0.044

KOH 1.289e-012 1.292e-012 -11.890 -11.889 0.001

Li 5.479e-006

Li+ 5.477e-006 4.976e-006 -5.261 -5.303 -0.042

LiSO4- 2.254e-009 2.038e-009 -8.647 -8.691 -0.044

LiOH 3.368e-012 3.376e-012 -11.473 -11.472 0.001

Mg 7.943e-004

Mg+2 7.470e-004 5.087e-004 -3.127 -3.293 -0.167

MgHCO3+ 3.673e-005 3.321e-005 -4.435 -4.479 -0.044

MgSO4 8.088e-006 8.106e-006 -5.092 -5.091 0.001

MgCO3 2.445e-006 2.451e-006 -5.612 -5.611 0.001

MgOH+ 1.956e-008 1.769e-008 -7.709 -7.752 -0.044

N(5) 3.072e-006

NO3- 3.072e-006 2.767e-006 -5.513 -5.558 -0.045

Na 2.098e-004

Na+ 2.091e-004 1.892e-004 -3.680 -3.723 -0.043

NaHCO3 6.151e-007 6.165e-007 -6.211 -6.210 0.001

NaSO4- 9.089e-008 8.217e-008 -7.042 -7.085 -0.044

NaCO3- 1.259e-008 1.138e-008 -7.900 -7.944 -0.044

NaOH 3.694e-011 3.702e-011 -10.433 -10.432 0.001

O(0) 5.792e-010

O2 2.896e-010 2.903e-010 -9.538 -9.537 0.001

S(6) 1.739e-004

SO4-2 1.392e-004 9.380e-005 -3.856 -4.028 -0.172

CaSO4 2.639e-005 2.645e-005 -4.579 -4.578 0.001

MgSO4 8.088e-006 8.106e-006 -5.092 -5.091 0.001

SrSO4 1.016e-007 1.018e-007 -6.993 -6.992 0.001

NaSO4- 9.089e-008 8.217e-008 -7.042 -7.085 -0.044

BaSO4 2.561e-008 2.567e-008 -7.592 -7.591 0.001

KSO4- 7.373e-009 6.666e-009 -8.132 -8.176 -0.044

LiSO4- 2.254e-009 2.038e-009 -8.647 -8.691 -0.044

HSO4- 2.657e-010 2.402e-010 -9.576 -9.619 -0.044

CaHSO4+ 5.073e-012 4.587e-012 -11.295 -11.338 -0.044

AlSO4+ 1.093e-012 9.881e-013 -11.961 -12.005 -0.044

Al(SO4)2- 3.059e-015 2.766e-015 -14.514 -14.558 -0.044

AlHSO4+2 4.061e-021 2.714e-021 -20.391 -20.566 -0.175

Si 1.099e-004

H4SiO4 1.096e-004 1.098e-004 -3.960 -3.959 0.001

H3SiO4- 3.375e-007 3.052e-007 -6.472 -6.515 -0.044

H2SiO4-2 3.973e-013 2.655e-013 -12.401 -12.576 -0.175

Sr 1.005e-005

Sr+2 9.512e-006 6.450e-006 -5.022 -5.190 -0.169

SrHCO3+ 4.179e-007 3.791e-007 -6.379 -6.421 -0.042

SrSO4 1.016e-007 1.018e-007 -6.993 -6.992 0.001

SrCO3 1.749e-008 1.753e-008 -7.757 -7.756 0.001

SrOH+ 1.081e-011 9.795e-012 -10.966 -11.009 -0.043

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -0.61 11.01 11.61 Al(OH)3

Albite -2.29 -21.09 -18.80 NaAlSi3O8

Alunite -2.49 -2.35 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.49 -6.83 -4.33 CaSO4

Anorthite -1.63 -21.70 -20.07 CaAl2Si2O8

Aragonite 0.25 -8.02 -8.27 CaCO3

Barite -0.11 -10.29 -10.18 BaSO4

Ca-Montmorillonite 4.09 -42.73 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.41 -8.02 -8.42 CaCO3

Celestite -2.59 -9.22 -6.62 SrSO4

Chalcedony -0.26 -3.96 -3.70 SiO2

Chlorite(14A) -4.65 68.38 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -6.72 27.03 33.75 Mg3Si2O5(OH)4

CO2(g) -1.96 -3.27 -1.31 CO2

Dolomite 0.27 -16.53 -16.80 CaMg(CO3)2

Gibbsite 2.20 11.01 8.81 Al(OH)3

Gypsum -2.24 -6.83 -4.59 CaSO4:2H2O

H2(g) -40.34 -43.44 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.64 -8.08 1.55 NaCl

Illite 2.73 -39.22 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -0.75 -22.27 -21.52 KAlSi3O8

K-mica 9.19 23.72 14.53 KAl3Si3O10(OH)2

Kaolinite 5.58 14.10 8.52 Al2Si2O5(OH)4

O2(g) -6.74 -9.54 -2.79 O2

Quartz 0.21 -3.96 -4.16 SiO2

Sepiolite -4.67 11.42 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -7.24 11.42 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.14 -3.96 -2.81 SiO2

Strontianite -1.13 -10.41 -9.28 SrCO3

Talc -3.71 19.11 22.82 Mg3Si4O10(OH)2

Witherite -2.87 -11.48 -8.61 BaCO3

------------------

End of simulation.

------------------

------------------------------------

Reading input data for simulation 2.

------------------------------------

-----------

End of run.

**Appendix. Geochemical model output of Well 4-6**

Input file: C:\Users\huan\Desktop\Phreeqc calculation Konza\4-6 Well\2006-09 4-6.pqi

Output file: C:\Users\huan\Desktop\Phreeqc calculation Konza\4-6 Well\2006-09 4-6.pqo

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

------------------

Reading data base.

------------------

SOLUTION\_MASTER\_SPECIES

SOLUTION\_SPECIES

PHASES

EXCHANGE\_MASTER\_SPECIES

EXCHANGE\_SPECIES

SURFACE\_MASTER\_SPECIES

SURFACE\_SPECIES

RATES

END

------------------------------------

Reading input data for simulation 1.

------------------------------------

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\phreeqc.dat

SOLUTION 1 06-4-2

temp 13

pH 7 Calcite 0.701

pe 12.7

redox pe

units ppm

density 1

Na 6.33

K 0.75

Ca 93.5

Mg 19.6

Sr 0.82

B 0.024

Ba 0.078

Li 0.023

Si 4.5

N(5) 0.019

S(6) 36.57

Cl 2.66

Alkalinity 340 as HCO3

water 1 # kg

SOLUTION 2 06-5-7

temp 13

pH 7 Calcite 0.54

pe 12.7

redox pe

units ppm

density 1

Na 7.08

K 0.75

Ca 92.2

Mg 21.2

Sr 0.97

Al 0.035

B 0.029

Ba 0.078

Li 0.023

Si 4.9

N(5) 0.016

S(6) 31.65

Cl 2.94

Alkalinity 361 as HCO3

water 1 # kg

SOLUTION 3 06-6-8

temp 13

pH 7 Calcite 0.348

pe 12.7

redox pe

units ppm

density 1

Na 5.38

K 0.94

Ca 96.4

Mg 21.8

Sr 1.11

Al 0.037

B 0.035

Ba 0.087

Li 0.027

Si 5.9

N(5) 0.021

S(6) 32.48

Cl 3.18

Alkalinity 378 as HCO3

water 1 # kg

SOLUTION 4 06-8-15

temp 13

pH 7 Calcite 0.027

pe 12.7

redox pe

units ppm

density 1

Na 7.16

K 1.03

Ca 98.2

Mg 20

Sr 0.87

B 0.038

Ba 0.095

Li 0.025

Si 5.7

N(5) 0.335

S(6) 53.46

Cl 3.66

Alkalinity 342 as HCO3

water 1 # kg

SOLUTION 5 06-9-24

temp 13

pH 7 Calcite -0.027

pe 12.7

redox pe

units ppm

density 1

Na 7.47

K 0.97

Ca 104.4

Mg 22.1

Sr 1

Al 0

B 0.036

Ba 0.093

Li 0.025

Si 5.6

N(5) 0.026

S(6) 37.08

Cl 2.98

Alkalinity 397 as HCO3

water 1 # kg

SOLUTION 6 06-10-12

temp 13

pH 7 Calcite -0.015

pe 12.7

redox pe

units ppm

density 1

Na 7.28

K 0.91

Ca 104.3

Mg 21.4

Sr 0.9

Al 0.007

B 0.034

Ba 0.106

Li 0.025

Si 5.6

N(5) 0.018

S(6) 34.77

Cl 3.22

Alkalinity 404 as HCO3

water 1 # kg

SOLUTION 7 06-11-18

temp 13

pH 7 Calcite 0.063

pe 12.7

redox pe

units ppm

density 1

Na 7.38

K 0.74

Ca 101.5

Mg 22.5

Sr 1.01

B 0.029

Ba 0.083

Li 0.025

Si 5.2

S(6) 42.4

Cl 3.92

Alkalinity 399 as HCO3

water 1 # kg

SOLUTION 8 07-1-4

temp 13

pH 7 Calcite 0.226

pe 12.7

redox pe

units ppm

density 1

Na 7.31

K 0.65

Ca 106.9

Mg 22

Sr 0.91

B 0.023

Ba 0.103

Li 0.023

Si 4.9

S(6) 47.17

Cl 3.05

Alkalinity 393 as HCO3

water 1 # kg

SOLUTION 9 07-2-18

temp 13

pH 7 Calcite 0.697

pe 12.7

redox pe

units ppm

density 1

Na 6.49

K 0.67

Ca 94

Mg 19.8

Sr 0.8

B 0.019

Ba 0.083

Li 0.022

Si 4

S(6) 44.18

Cl 2.42

Alkalinity 352.7 as HCO3

water 1 # kg

SOLUTION 10 07-3-18

temp 13

pH 7 Calcite 0.734

pe 12.7

redox pe

units ppm

density 1

Na 6.49

K 0.59

Ca 96.2

Mg 20.5

Sr 0.8

B 0.019

Ba 0.093

Li 0.02

Si 4.4

S(6) 37.54

Cl 2.72

Alkalinity 361.6 as HCO3

water 1 # kg

SOLUTION 11 07-4-22

temp 13

pH 7 Calcite 0.62

pe 12.7

redox pe

units ppm

density 1

Na 4.46

K 0.71

Ca 89

Mg 19

Sr 0.91

Al 0.003

B 0.029

Ba 0.09

Li 0.025

Si 5.1

S(6) 21.58

Cl 2.95

Alkalinity 351 as HCO3

water 1 # kg

SOLUTION 12 07-6-4

temp 13

pH 7 Calcite 0.372

pe 12.7

redox pe

units ppm

density 1

Na 4.77

K 0.83

Ca 87.6

Mg 20.3

Sr 1.03

B 0.034

Ba 0.089

Li 0.026

Si 5.8

N(5) 0.019

S(6) 20.38

Cl 2.59

Alkalinity 353 as HCO3

water 1 # kg

SOLUTION 13 07-7-24

temp 13

pH 7 Calcite 0.105

pe 12.7

redox pe

units ppm

density 1

Na 5.18

K 0.98

Ca 93.9

Mg 21.8

Sr 1.18

Al 0

B 0.041

Ba 0.089

Li 0.03

Si 6.2

N(5) 0.039

S(6) 30.44

Cl 3.04

Alkalinity 372 as HCO3

water 1 # kg

SOLUTION 14 07-8-26

temp 13

pH 7 Calcite 0.001

pe 12.7

redox pe

units ppm

density 1

Na 5.37

K 1.05

Ca 95.1

Mg 22.5

Sr 1.25

Al 0.013

B 0.043

Ba 0.083

Li 0.032

Si 6.6

N(5) 0.024

S(6) 34.91

Cl 2.82

Alkalinity 368 as HCO3

water 1 # kg

SOLUTION 15 07-9-22

temp 13

pH 7 Calcite -0.027

pe 12.7

redox pe

units ppm

density 1

Na 5.11

K 1.04

Ca 96.4

Mg 21.9

Sr 1.07

Al 0.04

B 0.057

Ba 0.094

Li 0.031

Si 6.1

N(5) 0.053

S(6) 36.11

Cl 2.71

Alkalinity 374 as HCO3

water 1 # kg

SOLUTION 16 07-10-28

temp 13

pH 7 Calcite -0.011

pe 12.7

redox pe

units ppm

density 1

Na 5.36

K 1.1

Ca 100.8

Mg 23.4

Sr 1.19

Al 0.25

B 0.042

Ba 0.094

Li 0.03

Si 6.7

N(5) 0.022

S(6) 44.31

Cl 2.97

Alkalinity 374 as HCO3

water 1 # kg

SOLUTION 17 07-11-18

temp 13

pH 7 Calcite 0.063

pe 12.7

redox pe

units ppm

density 1

Na 5.44

K 0.98

Ca 99.5

Mg 23.5

Sr 1.19

B 0.041

Ba 0.091

Li 0.03

Si 6

S(6) 44.33

Cl 2.7

Alkalinity 384 as HCO3

water 1 # kg

SOLUTION 18 08-4-6

temp 13

pH 7 calcite 0.684

pe 12.7

redox pe

units ppm

density 1

Na 4.22

K 0.85

Ca 87.4

Mg 18.6

Sr 0.79

Al 0.061

B 0.021

Ba 0.088

Li 0.026

Si 4.78

S(6) 19.92

Cl 2.23

Alkalinity 348 as HCO3

water 1 # kg

SOLUTION 19 08-5-20

temp 13

pH 7 Calcite 0.457

pe 12.7

redox pe

units ppm

density 1

Na 4.64

K 0.9

Ca 91.9

Mg 20.6

Sr 0.98

B 0.026

Ba 0.089

Li 0.029

Si 5.25

S(6) 24.12

Cl 2.96

Alkalinity 362 as HCO3

water 1 # kg

SOLUTION 20 08-6-21

temp 13

pH 7 Calcite 0.266

pe 12.7

redox pe

units ppm

density 1

Na 5.11

K 0.97

Ca 92.7

Mg 21.8

Sr 1.09

B 0.032

Ba 0.088

Li 0.033

Si 5.66

N(5) 0.084

S(6) 23.02

Cl 3.16

Alkalinity 381 as HCO3

water 1 # kg

SOLUTION 21 08-8-7

temp 13

pH 7 Calcite 0.049

pe 12.7

redox pe

units ppm

density 1

Na 5.09

K 1.01

Ca 90.1

Mg 22.8

Sr 1.23

Al 0

B 0.037

Ba 0.081

Li 0.034

Si 5.98

N(5) 0.038

S(6) 27.46

Cl 3.03

Alkalinity 381 as HCO3

water 1 # kg

SOLUTION 22 08-9-21

temp 13

pH 7 Calcite -0.027

pe 12.7

redox pe

units ppm

density 1

Na 4.75

K 0.99

Ca 88.3

Mg 19.9

Sr 1.04

Al 0.01

B 0.033

Ba 0.091

Li 0.047

Si 5.99

N(5) 0.038

S(6) 20.67

Cl 2.52

Alkalinity 382 as HCO3

water 1 # kg

SOLUTION 23 08-11-2

temp 13

pH 7 Calcite 0.024

pe 12.7

redox pe

units ppm

density 1

Na 5.33

K 1.05

Ca 90.7

Mg 22.6

Sr 1.19

Al 0.135

B 0.03

Ba 0.087

Li 0.03

Si 6.15

N(5) 0.069

S(6) 29.05

Cl 2.31

Alkalinity 367 as HCO3

water 1 # kg

SOLUTION 24 08-11-30

temp 13

pH 7 Calcite 0.101

pe 12.7

redox pe

units ppm

density 1

Na 5.31

K 1.19

Ca 92.3

Mg 23.8

Sr 1.22

Al 0.779

B 0.033

Ba 0.084

Li 0.046

Si 7.44

N(5) 0.078

S(6) 30.5

Cl 3.67

Alkalinity 376 as HCO3

water 1 # kg

SOLUTION 25 09-1-6

temp 13

pH 7 Calcite 0.261

pe 12.7

redox pe

units ppm

density 1

Na 4.39

K 0.38

Ca 85.9

Mg 19.1

Sr 0.94

Al 0.037

B 0.02

Ba 0.084

Li 0.011

Si 4.88

N(5) 0.025

S(6) 28.77

Cl 2.23

Alkalinity 362 as HCO3

water 1 # kg

SOLUTION 26 09-2-21

temp 13

pH 7 Calcite 0.708

pe 12.7

redox pe

units ppm

density 1

Na 4.37

K 0.47

Ca 92.5

Mg 19.9

Sr 0.88

Al 0.386

B 0.019

Ba 0.087

Li 0.037

Si 5.53

N(5) 0.027

S(6) 33.94

Cl 2.2

Alkalinity 351 as HCO3

water 1 # kg

SOLUTION 27 09-4-18

temp 13

pH 7 Calcite 0.639

pe 12.7

redox pe

units ppm

density 1

Na 4.24

K 0.44

Ca 88.9

Mg 18.6

Sr 0.85

Al 0.015

B 0.021

Ba 0.087

Li 0.036

Si 5

S(6) 18.78

Cl 2.18

Alkalinity 359 as HCO3

water 1 # kg

SOLUTION 28 09-5-20

temp 13

pH 7 Calcite 0.463

pe 12.7

redox pe

units ppm

density 1

Na 4.69

K 0.5

Ca 91.4

Mg 19.1

Sr 0.93

B 0.026

Ba 0.092

Li 0.036

Si 5.4

N(5) 0.03

S(6) 19.33

Cl 1.99

Alkalinity 376 as HCO3

water 1 # kg

SOLUTION 29 09-7-7

temp 13

pH 7 Calcite 0.184

pe 12.7

redox pe

units ppm

density 1

Na 5.67

K 0.57

Ca 93.3

Mg 22.6

Sr 1.23

Al 0.045

B 0.033

Ba 0.084

Li 0.039

Si 6.07

N(5) 0.024

S(6) 27.82

Cl 2.5

Alkalinity 392 as HCO3

water 1 # kg

SELECTED\_OUTPUT

file C:\Users\huan\Desktop\2006-09 4-6 selected.out.sel

reset false

ph true

pe true

temperature true

alkalinity true

ionic\_strength true

percent\_error true

molalities Ca+2 Mg+2

saturation\_indices CO2(g) Calcite Aragonite Dolomite

Quartz Chalcedony

-------------------------------------------

Beginning of initial solution calculations.

-------------------------------------------

Initial solution 1. 06-4-2

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 5.575e-003 5.575e-003

B 2.221e-006 2.221e-006

Ba 5.682e-007 5.682e-007

Ca 2.334e-003 2.334e-003

Cl 7.507e-005 7.507e-005

K 1.919e-005 1.919e-005

Li 3.316e-006 3.316e-006

Mg 8.066e-004 8.066e-004

N(5) 1.357e-006 1.357e-006

Na 2.755e-004 2.755e-004

S(6) 3.809e-004 3.809e-004

Si 7.493e-005 7.493e-005

Sr 9.363e-006 9.363e-006

----------------------------Description of solution----------------------------

pH = 7.872 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 431

Density (g/cm3) = 0.99980

Activity of water = 1.000

Ionic strength = 9.443e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 5.701e-003

Total CO2 (mol/kg) = 5.701e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = 1.860e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 1.50

Iterations = 9

Total H = 1.110182e+002

Total O = 5.552498e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.130e-007 2.830e-007 -6.504 -6.548 -0.044

H+ 1.465e-008 1.343e-008 -7.834 -7.872 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 2.221e-006

H3BO3 2.141e-006 2.145e-006 -5.669 -5.669 0.001

H2BO3- 8.074e-008 7.315e-008 -7.093 -7.136 -0.043

Ba 5.682e-007

Ba+2 5.173e-007 3.516e-007 -6.286 -6.454 -0.168

BaSO4 3.670e-008 3.678e-008 -7.435 -7.434 0.001

BaHCO3+ 1.242e-008 1.126e-008 -7.906 -7.949 -0.043

BaCO3 1.827e-009 1.831e-009 -8.738 -8.737 0.001

BaOH+ 9.788e-013 8.869e-013 -12.009 -12.052 -0.043

C(4) 5.701e-003

HCO3- 5.360e-003 4.872e-003 -2.271 -2.312 -0.041

CO2 1.781e-004 1.785e-004 -3.749 -3.748 0.001

CaHCO3+ 7.994e-005 7.266e-005 -4.097 -4.139 -0.041

MgHCO3+ 3.126e-005 2.833e-005 -4.505 -4.548 -0.043

CaCO3 2.656e-005 2.662e-005 -4.576 -4.575 0.001

CO3-2 1.879e-005 1.283e-005 -4.726 -4.892 -0.166

MgCO3 5.242e-006 5.253e-006 -5.281 -5.280 0.001

NaHCO3 6.807e-007 6.822e-007 -6.167 -6.166 0.001

SrHCO3+ 3.267e-007 2.969e-007 -6.486 -6.527 -0.041

NaCO3- 3.494e-008 3.166e-008 -7.457 -7.500 -0.043

SrCO3 3.445e-008 3.452e-008 -7.463 -7.462 0.001

BaHCO3+ 1.242e-008 1.126e-008 -7.906 -7.949 -0.043

BaCO3 1.827e-009 1.831e-009 -8.738 -8.737 0.001

Ca 2.334e-003

Ca+2 2.173e-003 1.482e-003 -2.663 -2.829 -0.166

CaHCO3+ 7.994e-005 7.266e-005 -4.097 -4.139 -0.041

CaSO4 5.480e-005 5.492e-005 -4.261 -4.260 0.001

CaCO3 2.656e-005 2.662e-005 -4.576 -4.575 0.001

CaOH+ 2.021e-008 1.831e-008 -7.694 -7.737 -0.043

CaHSO4+ 4.182e-012 3.789e-012 -11.379 -11.421 -0.043

Cl 7.507e-005

Cl- 7.507e-005 6.790e-005 -4.125 -4.168 -0.044

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -44.241 -44.240 0.001

K 1.919e-005

K+ 1.917e-005 1.734e-005 -4.717 -4.761 -0.044

KSO4- 2.256e-008 2.044e-008 -7.647 -7.689 -0.043

KOH 4.465e-012 4.475e-012 -11.350 -11.349 0.001

Li 3.316e-006

Li+ 3.313e-006 3.016e-006 -5.480 -5.521 -0.041

LiSO4- 3.033e-009 2.748e-009 -8.518 -8.561 -0.043

LiOH 5.132e-012 5.143e-012 -11.290 -11.289 0.001

Mg 8.066e-004

Mg+2 7.518e-004 5.160e-004 -3.124 -3.287 -0.163

MgHCO3+ 3.126e-005 2.833e-005 -4.505 -4.548 -0.043

MgSO4 1.825e-005 1.829e-005 -4.739 -4.738 0.001

MgCO3 5.242e-006 5.253e-006 -5.281 -5.280 0.001

MgOH+ 4.976e-008 4.509e-008 -7.303 -7.346 -0.043

N(5) 1.357e-006

NO3- 1.357e-006 1.225e-006 -5.867 -5.912 -0.044

Na 2.755e-004

Na+ 2.745e-004 2.490e-004 -3.561 -3.604 -0.042

NaHCO3 6.807e-007 6.822e-007 -6.167 -6.166 0.001

NaSO4- 2.655e-007 2.406e-007 -6.576 -6.619 -0.043

NaCO3- 3.494e-008 3.166e-008 -7.457 -7.500 -0.043

NaOH 1.222e-010 1.224e-010 -9.913 -9.912 0.001

O(0) 2.313e-008

O2 1.156e-008 1.159e-008 -7.937 -7.936 0.001

S(6) 3.809e-004

SO4-2 3.073e-004 2.087e-004 -3.512 -3.680 -0.168

CaSO4 5.480e-005 5.492e-005 -4.261 -4.260 0.001

MgSO4 1.825e-005 1.829e-005 -4.739 -4.738 0.001

NaSO4- 2.655e-007 2.406e-007 -6.576 -6.619 -0.043

SrSO4 2.106e-007 2.110e-007 -6.677 -6.676 0.001

BaSO4 3.670e-008 3.678e-008 -7.435 -7.434 0.001

KSO4- 2.256e-008 2.044e-008 -7.647 -7.689 -0.043

LiSO4- 3.033e-009 2.748e-009 -8.518 -8.561 -0.043

HSO4- 2.347e-010 2.126e-010 -9.630 -9.672 -0.043

CaHSO4+ 4.182e-012 3.789e-012 -11.379 -11.421 -0.043

Si 7.493e-005

H4SiO4 7.436e-005 7.452e-005 -4.129 -4.128 0.001

H3SiO4- 5.745e-007 5.205e-007 -6.241 -6.284 -0.043

H2SiO4-2 1.689e-012 1.139e-012 -11.772 -11.944 -0.171

Sr 9.363e-006

Sr+2 8.792e-006 6.008e-006 -5.056 -5.221 -0.165

SrHCO3+ 3.267e-007 2.969e-007 -6.486 -6.527 -0.041

SrSO4 2.106e-007 2.110e-007 -6.677 -6.676 0.001

SrCO3 3.445e-008 3.452e-008 -7.463 -7.462 0.001

SrOH+ 2.526e-011 2.294e-011 -10.598 -10.639 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.18 -6.51 -4.33 CaSO4

Aragonite 0.55 -7.72 -8.27 CaCO3

Barite 0.05 -10.13 -10.18 BaSO4

Calcite 0.70 -7.72 -8.42 CaCO3

Celestite -2.28 -8.90 -6.62 SrSO4

Chalcedony -0.43 -4.13 -3.70 SiO2

Chrysotile -4.64 29.11 33.75 Mg3Si2O5(OH)4

CO2(g) -2.44 -3.75 -1.31 CO2

Dolomite 0.90 -15.90 -16.80 CaMg(CO3)2

Gypsum -1.92 -6.51 -4.59 CaSO4:2H2O

H2(g) -41.14 -44.24 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.33 -7.77 1.55 NaCl

O2(g) -5.14 -7.94 -2.79 O2

Quartz 0.04 -4.13 -4.16 SiO2

Sepiolite -3.56 12.53 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -6.13 12.53 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.31 -4.13 -2.81 SiO2

Strontianite -0.83 -10.11 -9.28 SrCO3

Talc -1.97 20.86 22.82 Mg3Si4O10(OH)2

Witherite -2.74 -11.35 -8.61 BaCO3

Initial solution 2. 06-5-7

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 1.298e-006 1.298e-006

Alkalinity 5.919e-003 5.919e-003

B 2.684e-006 2.684e-006

Ba 5.682e-007 5.682e-007

Ca 2.302e-003 2.302e-003

Cl 8.297e-005 8.297e-005

K 1.919e-005 1.919e-005

Li 3.316e-006 3.316e-006

Mg 8.725e-004 8.725e-004

N(5) 1.143e-006 1.143e-006

Na 3.081e-004 3.081e-004

S(6) 3.296e-004 3.296e-004

Si 8.159e-005 8.159e-005

Sr 1.108e-005 1.108e-005

----------------------------Description of solution----------------------------

pH = 7.689 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 441

Density (g/cm3) = 0.99981

Activity of water = 1.000

Ionic strength = 9.644e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.168e-003

Total CO2 (mol/kg) = 6.168e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = 4.326e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.34

Iterations = 10

Total H = 1.110186e+002

Total O = 5.552609e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.054e-007 1.856e-007 -6.687 -6.731 -0.044

H+ 2.236e-008 2.049e-008 -7.650 -7.689 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 1.298e-006

Al(OH)4- 1.278e-006 1.157e-006 -5.893 -5.937 -0.043

Al(OH)3 1.415e-008 1.418e-008 -7.849 -7.848 0.001

Al(OH)2+ 5.684e-009 5.146e-009 -8.245 -8.289 -0.043

AlOH+2 6.179e-011 4.150e-011 -10.209 -10.382 -0.173

Al+3 4.199e-013 1.907e-013 -12.377 -12.720 -0.343

AlSO4+ 1.018e-013 9.217e-014 -12.992 -13.035 -0.043

Al(SO4)2- 5.460e-016 4.943e-016 -15.263 -15.306 -0.043

AlHSO4+2 2.287e-022 1.536e-022 -21.641 -21.814 -0.173

B 2.684e-006

H3BO3 2.619e-006 2.625e-006 -5.582 -5.581 0.001

H2BO3- 6.483e-008 5.869e-008 -7.188 -7.231 -0.043

Ba 5.682e-007

Ba+2 5.218e-007 3.535e-007 -6.282 -6.452 -0.169

BaSO4 3.177e-008 3.184e-008 -7.498 -7.497 0.001

BaHCO3+ 1.333e-008 1.207e-008 -7.875 -7.918 -0.043

BaCO3 1.284e-009 1.287e-009 -8.891 -8.890 0.001

BaOH+ 6.457e-013 5.846e-013 -12.190 -12.233 -0.043

C(4) 6.168e-003

HCO3- 5.721e-003 5.196e-003 -2.243 -2.284 -0.042

CO2 2.896e-004 2.903e-004 -3.538 -3.537 0.001

CaHCO3+ 8.423e-005 7.649e-005 -4.075 -4.116 -0.042

MgHCO3+ 3.607e-005 3.265e-005 -4.443 -4.486 -0.043

CaCO3 1.833e-005 1.837e-005 -4.737 -4.736 0.001

CO3-2 1.318e-005 8.969e-006 -4.880 -5.047 -0.167

MgCO3 3.961e-006 3.970e-006 -5.402 -5.401 0.001

NaHCO3 8.111e-007 8.129e-007 -6.091 -6.090 0.001

SrHCO3+ 4.119e-007 3.741e-007 -6.385 -6.427 -0.042

SrCO3 2.845e-008 2.851e-008 -7.546 -7.545 0.001

NaCO3- 2.732e-008 2.473e-008 -7.563 -7.607 -0.043

BaHCO3+ 1.333e-008 1.207e-008 -7.875 -7.918 -0.043

BaCO3 1.284e-009 1.287e-009 -8.891 -8.890 0.001

Ca 2.302e-003

Ca+2 2.152e-003 1.463e-003 -2.667 -2.835 -0.168

CaHCO3+ 8.423e-005 7.649e-005 -4.075 -4.116 -0.042

CaSO4 4.659e-005 4.669e-005 -4.332 -4.331 0.001

CaCO3 1.833e-005 1.837e-005 -4.737 -4.736 0.001

CaOH+ 1.309e-008 1.185e-008 -7.883 -7.926 -0.043

CaHSO4+ 5.427e-012 4.913e-012 -11.265 -11.309 -0.043

Cl 8.297e-005

Cl- 8.297e-005 7.498e-005 -4.081 -4.125 -0.044

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.874 -43.873 0.001

K 1.919e-005

K+ 1.917e-005 1.733e-005 -4.717 -4.761 -0.044

KSO4- 1.943e-008 1.759e-008 -7.712 -7.755 -0.043

KOH 2.925e-012 2.932e-012 -11.534 -11.533 0.001

Li 3.316e-006

Li+ 3.314e-006 3.014e-006 -5.480 -5.521 -0.041

LiSO4- 2.612e-009 2.365e-009 -8.583 -8.626 -0.043

LiOH 3.362e-012 3.370e-012 -11.473 -11.472 0.001

Mg 8.725e-004

Mg+2 8.154e-004 5.577e-004 -3.089 -3.254 -0.165

MgHCO3+ 3.607e-005 3.265e-005 -4.443 -4.486 -0.043

MgSO4 1.699e-005 1.703e-005 -4.770 -4.769 0.001

MgCO3 3.961e-006 3.970e-006 -5.402 -5.401 0.001

MgOH+ 3.530e-008 3.196e-008 -7.452 -7.495 -0.043

N(5) 1.143e-006

NO3- 1.143e-006 1.031e-006 -5.942 -5.987 -0.045

Na 3.081e-004

Na+ 3.070e-004 2.782e-004 -3.513 -3.556 -0.043

NaHCO3 8.111e-007 8.129e-007 -6.091 -6.090 0.001

NaSO4- 2.557e-007 2.315e-007 -6.592 -6.635 -0.043

NaCO3- 2.732e-008 2.473e-008 -7.563 -7.607 -0.043

NaOH 8.951e-011 8.971e-011 -10.048 -10.047 0.001

O(0) 4.273e-009

O2 2.137e-009 2.141e-009 -8.670 -8.669 0.001

S(6) 3.296e-004

SO4-2 2.655e-004 1.797e-004 -3.576 -3.745 -0.170

CaSO4 4.659e-005 4.669e-005 -4.332 -4.331 0.001

MgSO4 1.699e-005 1.703e-005 -4.770 -4.769 0.001

NaSO4- 2.557e-007 2.315e-007 -6.592 -6.635 -0.043

SrSO4 2.142e-007 2.147e-007 -6.669 -6.668 0.001

BaSO4 3.177e-008 3.184e-008 -7.498 -7.497 0.001

KSO4- 1.943e-008 1.759e-008 -7.712 -7.755 -0.043

LiSO4- 2.612e-009 2.365e-009 -8.583 -8.626 -0.043

HSO4- 3.085e-010 2.792e-010 -9.511 -9.554 -0.043

CaHSO4+ 5.427e-012 4.913e-012 -11.265 -11.309 -0.043

AlSO4+ 1.018e-013 9.217e-014 -12.992 -13.035 -0.043

Al(SO4)2- 5.460e-016 4.943e-016 -15.263 -15.306 -0.043

AlHSO4+2 2.287e-022 1.536e-022 -21.641 -21.814 -0.173

Si 8.159e-005

H4SiO4 8.118e-005 8.136e-005 -4.091 -4.090 0.001

H3SiO4- 4.116e-007 3.726e-007 -6.385 -6.429 -0.043

H2SiO4-2 7.957e-013 5.344e-013 -12.099 -12.272 -0.173

Sr 1.108e-005

Sr+2 1.042e-005 7.098e-006 -4.982 -5.149 -0.167

SrHCO3+ 4.119e-007 3.741e-007 -6.385 -6.427 -0.042

SrSO4 2.142e-007 2.147e-007 -6.669 -6.668 0.001

SrCO3 2.845e-008 2.851e-008 -7.546 -7.545 0.001

SrOH+ 1.958e-011 1.777e-011 -10.708 -10.750 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -1.27 10.35 11.61 Al(OH)3

Albite -2.96 -21.76 -18.80 NaAlSi3O8

Alunite -4.42 -4.28 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.25 -6.58 -4.33 CaSO4

Anorthite -2.82 -22.89 -20.07 CaAl2Si2O8

Aragonite 0.39 -7.88 -8.27 CaCO3

Barite -0.01 -10.20 -10.18 BaSO4

Ca-Montmorillonite 2.14 -44.69 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.54 -7.88 -8.42 CaCO3

Celestite -2.27 -8.89 -6.62 SrSO4

Chalcedony -0.39 -4.09 -3.70 SiO2

Chlorite(14A) -4.00 69.04 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -5.56 28.19 33.75 Mg3Si2O5(OH)4

CO2(g) -2.22 -3.54 -1.31 CO2

Dolomite 0.62 -16.18 -16.80 CaMg(CO3)2

Gibbsite 1.53 10.35 8.81 Al(OH)3

Gypsum -1.99 -6.58 -4.59 CaSO4:2H2O

H2(g) -40.78 -43.87 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.23 -7.68 1.55 NaCl

Illite 1.08 -40.86 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -1.45 -22.97 -21.52 KAlSi3O8

K-mica 7.17 21.70 14.53 KAl3Si3O10(OH)2

Kaolinite 3.99 12.51 8.52 Al2Si2O5(OH)4

O2(g) -5.88 -8.67 -2.79 O2

Quartz 0.08 -4.09 -4.16 SiO2

Sepiolite -4.11 11.98 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -6.68 11.98 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.27 -4.09 -2.81 SiO2

Strontianite -0.92 -10.20 -9.28 SrCO3

Talc -2.81 20.01 22.82 Mg3Si4O10(OH)2

Witherite -2.89 -11.50 -8.61 BaCO3

Initial solution 3. 06-6-8

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 1.372e-006 1.372e-006

Alkalinity 6.198e-003 6.198e-003

B 3.240e-006 3.240e-006

Ba 6.338e-007 6.338e-007

Ca 2.407e-003 2.407e-003

Cl 8.975e-005 8.975e-005

K 2.405e-005 2.405e-005

Li 3.893e-006 3.893e-006

Mg 8.972e-004 8.972e-004

N(5) 1.500e-006 1.500e-006

Na 2.341e-004 2.341e-004

S(6) 3.383e-004 3.383e-004

Si 9.825e-005 9.825e-005

Sr 1.268e-005 1.268e-005

----------------------------Description of solution----------------------------

pH = 7.458 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 457

Density (g/cm3) = 0.99983

Activity of water = 1.000

Ionic strength = 1.002e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.686e-003

Total CO2 (mol/kg) = 6.686e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -6.583e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.50

Iterations = 10

Total H = 1.110190e+002

Total O = 5.552753e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.211e-007 1.092e-007 -6.917 -6.962 -0.045

H+ 3.806e-008 3.482e-008 -7.420 -7.458 -0.039

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 1.372e-006

Al(OH)4- 1.330e-006 1.202e-006 -5.876 -5.920 -0.044

Al(OH)3 2.498e-008 2.504e-008 -7.602 -7.601 0.001

Al(OH)2+ 1.708e-008 1.544e-008 -7.767 -7.811 -0.044

AlOH+2 3.171e-010 2.115e-010 -9.499 -9.675 -0.176

Al+3 3.681e-012 1.652e-012 -11.434 -11.782 -0.348

AlSO4+ 8.960e-013 8.098e-013 -12.048 -12.092 -0.044

Al(SO4)2- 4.873e-015 4.404e-015 -14.312 -14.356 -0.044

AlHSO4+2 3.438e-021 2.293e-021 -20.464 -20.640 -0.176

B 3.240e-006

H3BO3 3.193e-006 3.200e-006 -5.496 -5.495 0.001

H2BO3- 4.659e-008 4.210e-008 -7.332 -7.376 -0.044

Ba 6.338e-007

Ba+2 5.817e-007 3.915e-007 -6.235 -6.407 -0.172

BaSO4 3.568e-008 3.576e-008 -7.448 -7.447 0.001

BaHCO3+ 1.553e-008 1.403e-008 -7.809 -7.853 -0.044

BaCO3 8.787e-010 8.807e-010 -9.056 -9.055 0.001

BaOH+ 4.216e-013 3.810e-013 -12.375 -12.419 -0.044

C(4) 6.686e-003

HCO3- 6.015e-003 5.454e-003 -2.221 -2.263 -0.043

CO2 5.167e-004 5.179e-004 -3.287 -3.286 0.001

CaHCO3+ 9.214e-005 8.355e-005 -4.036 -4.078 -0.043

MgHCO3+ 3.876e-005 3.503e-005 -4.412 -4.456 -0.044

CaCO3 1.178e-005 1.181e-005 -4.929 -4.928 0.001

CO3-2 8.196e-006 5.541e-006 -5.086 -5.256 -0.170

MgCO3 2.500e-006 2.506e-006 -5.602 -5.601 0.001

NaHCO3 6.459e-007 6.474e-007 -6.190 -6.189 0.001

SrHCO3+ 4.921e-007 4.462e-007 -6.308 -6.350 -0.043

SrCO3 1.997e-008 2.002e-008 -7.700 -7.699 0.001

BaHCO3+ 1.553e-008 1.403e-008 -7.809 -7.853 -0.044

NaCO3- 1.283e-008 1.159e-008 -7.892 -7.936 -0.044

BaCO3 8.787e-010 8.807e-010 -9.056 -9.055 0.001

Ca 2.407e-003

Ca+2 2.253e-003 1.522e-003 -2.647 -2.817 -0.170

CaHCO3+ 9.214e-005 8.355e-005 -4.036 -4.078 -0.043

CaSO4 4.915e-005 4.926e-005 -4.309 -4.308 0.001

CaCO3 1.178e-005 1.181e-005 -4.929 -4.928 0.001

CaOH+ 8.029e-009 7.256e-009 -8.095 -8.139 -0.044

CaHSO4+ 9.747e-012 8.809e-012 -11.011 -11.055 -0.044

Cl 8.975e-005

Cl- 8.975e-005 8.096e-005 -4.047 -4.092 -0.045

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.413 -43.412 0.001

K 2.405e-005

K+ 2.403e-005 2.168e-005 -4.619 -4.664 -0.045

KSO4- 2.469e-008 2.232e-008 -7.607 -7.651 -0.044

KOH 2.153e-012 2.158e-012 -11.667 -11.666 0.001

Li 3.893e-006

Li+ 3.890e-006 3.533e-006 -5.410 -5.452 -0.042

LiSO4- 3.110e-009 2.811e-009 -8.507 -8.551 -0.044

LiOH 2.319e-012 2.324e-012 -11.635 -11.634 0.001

Mg 8.972e-004

Mg+2 8.383e-004 5.699e-004 -3.077 -3.244 -0.168

MgHCO3+ 3.876e-005 3.503e-005 -4.412 -4.456 -0.044

MgSO4 1.760e-005 1.765e-005 -4.754 -4.753 0.001

MgCO3 2.500e-006 2.506e-006 -5.602 -5.601 0.001

MgOH+ 2.126e-008 1.921e-008 -7.672 -7.716 -0.044

N(5) 1.500e-006

NO3- 1.500e-006 1.351e-006 -5.824 -5.869 -0.046

Na 2.341e-004

Na+ 2.333e-004 2.111e-004 -3.632 -3.676 -0.043

NaHCO3 6.459e-007 6.474e-007 -6.190 -6.189 0.001

NaSO4- 1.971e-007 1.781e-007 -6.705 -6.749 -0.044

NaCO3- 1.283e-008 1.159e-008 -7.892 -7.936 -0.044

NaOH 3.995e-011 4.005e-011 -10.398 -10.397 0.001

O(0) 5.123e-010

O2 2.562e-010 2.567e-010 -9.591 -9.590 0.001

S(6) 3.383e-004

SO4-2 2.710e-004 1.823e-004 -3.567 -3.739 -0.172

CaSO4 4.915e-005 4.926e-005 -4.309 -4.308 0.001

MgSO4 1.760e-005 1.765e-005 -4.754 -4.753 0.001

SrSO4 2.468e-007 2.474e-007 -6.608 -6.607 0.001

NaSO4- 1.971e-007 1.781e-007 -6.705 -6.749 -0.044

BaSO4 3.568e-008 3.576e-008 -7.448 -7.447 0.001

KSO4- 2.469e-008 2.232e-008 -7.607 -7.651 -0.044

LiSO4- 3.110e-009 2.811e-009 -8.507 -8.551 -0.044

HSO4- 5.325e-010 4.813e-010 -9.274 -9.318 -0.044

CaHSO4+ 9.747e-012 8.809e-012 -11.011 -11.055 -0.044

AlSO4+ 8.960e-013 8.098e-013 -12.048 -12.092 -0.044

Al(SO4)2- 4.873e-015 4.404e-015 -14.312 -14.356 -0.044

AlHSO4+2 3.438e-021 2.293e-021 -20.464 -20.640 -0.176

Si 9.825e-005

H4SiO4 9.796e-005 9.818e-005 -4.009 -4.008 0.001

H3SiO4- 2.928e-007 2.646e-007 -6.533 -6.577 -0.044

H2SiO4-2 3.347e-013 2.233e-013 -12.475 -12.651 -0.176

Sr 1.268e-005

Sr+2 1.192e-005 8.066e-006 -4.924 -5.093 -0.169

SrHCO3+ 4.921e-007 4.462e-007 -6.308 -6.350 -0.043

SrSO4 2.468e-007 2.474e-007 -6.608 -6.607 0.001

SrCO3 1.997e-008 2.002e-008 -7.700 -7.699 0.001

SrOH+ 1.312e-011 1.188e-011 -10.882 -10.925 -0.043

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -1.02 10.59 11.61 Al(OH)3

Albite -2.82 -21.62 -18.80 NaAlSi3O8

Alunite -2.88 -2.74 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.22 -6.56 -4.33 CaSO4

Anorthite -2.60 -22.67 -20.07 CaAl2Si2O8

Aragonite 0.20 -8.07 -8.27 CaCO3

Barite 0.04 -10.15 -10.18 BaSO4

Ca-Montmorillonite 2.94 -43.88 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.35 -8.07 -8.42 CaCO3

Celestite -2.21 -8.83 -6.62 SrSO4

Chalcedony -0.31 -4.01 -3.70 SiO2

Chlorite(14A) -5.51 67.52 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -6.75 27.00 33.75 Mg3Si2O5(OH)4

CO2(g) -1.97 -3.29 -1.31 CO2

Dolomite 0.23 -16.57 -16.80 CaMg(CO3)2

Gibbsite 1.78 10.59 8.81 Al(OH)3

Gypsum -1.97 -6.56 -4.59 CaSO4:2H2O

H2(g) -40.32 -43.41 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.32 -7.77 1.55 NaCl

Illite 1.75 -40.20 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -1.09 -22.61 -21.52 KAlSi3O8

K-mica 8.02 22.55 14.53 KAl3Si3O10(OH)2

Kaolinite 4.65 13.17 8.52 Al2Si2O5(OH)4

O2(g) -6.80 -9.59 -2.79 O2

Quartz 0.16 -4.01 -4.16 SiO2

Sepiolite -4.77 11.32 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -7.34 11.32 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.19 -4.01 -2.81 SiO2

Strontianite -1.07 -10.35 -9.28 SrCO3

Talc -3.84 18.99 22.82 Mg3Si4O10(OH)2

Witherite -3.05 -11.66 -8.61 BaCO3

Initial solution 4. 06-8-15

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 5.608e-003 5.608e-003

B 3.517e-006 3.517e-006

Ba 6.921e-007 6.921e-007

Ca 2.451e-003 2.451e-003

Cl 1.033e-004 1.033e-004

K 2.636e-005 2.636e-005

Li 3.605e-006 3.605e-006

Mg 8.231e-004 8.231e-004

N(5) 2.393e-005 2.393e-005

Na 3.116e-004 3.116e-004

S(6) 5.568e-004 5.568e-004

Si 9.492e-005 9.492e-005

Sr 9.935e-006 9.935e-006

----------------------------Description of solution----------------------------

pH = 7.174 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 459

Density (g/cm3) = 0.99983

Activity of water = 1.000

Ionic strength = 1.003e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.501e-003

Total CO2 (mol/kg) = 6.501e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = 6.318e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.48

Iterations = 9

Total H = 1.110184e+002

Total O = 5.552751e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

H+ 7.325e-008 6.701e-008 -7.135 -7.174 -0.039

OH- 6.291e-008 5.673e-008 -7.201 -7.246 -0.045

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 3.517e-006

H3BO3 3.491e-006 3.499e-006 -5.457 -5.456 0.001

H2BO3- 2.646e-008 2.391e-008 -7.577 -7.621 -0.044

Ba 6.921e-007

Ba+2 6.145e-007 4.135e-007 -6.211 -6.384 -0.172

BaSO4 6.219e-008 6.234e-008 -7.206 -7.205 0.001

BaHCO3+ 1.491e-008 1.347e-008 -7.827 -7.871 -0.044

BaCO3 4.383e-010 4.393e-010 -9.358 -9.357 0.001

BaOH+ 2.313e-013 2.090e-013 -12.636 -12.680 -0.044

C(4) 6.501e-003

HCO3- 5.469e-003 4.958e-003 -2.262 -2.305 -0.043

CO2 9.041e-004 9.062e-004 -3.044 -3.043 0.001

CaHCO3+ 8.469e-005 7.679e-005 -4.072 -4.115 -0.043

MgHCO3+ 3.208e-005 2.899e-005 -4.494 -4.538 -0.044

CaCO3 5.626e-006 5.639e-006 -5.250 -5.249 0.001

CO3-2 3.872e-006 2.617e-006 -5.412 -5.582 -0.170

MgCO3 1.075e-006 1.078e-006 -5.969 -5.967 0.001

NaHCO3 7.811e-007 7.829e-007 -6.107 -6.106 0.001

SrHCO3+ 3.477e-007 3.152e-007 -6.459 -6.501 -0.043

BaHCO3+ 1.491e-008 1.347e-008 -7.827 -7.871 -0.044

NaCO3- 8.059e-009 7.283e-009 -8.094 -8.138 -0.044

SrCO3 7.329e-009 7.346e-009 -8.135 -8.134 0.001

BaCO3 4.383e-010 4.393e-010 -9.358 -9.357 0.001

Ca 2.451e-003

Ca+2 2.279e-003 1.539e-003 -2.642 -2.813 -0.170

CaHCO3+ 8.469e-005 7.679e-005 -4.072 -4.115 -0.043

CaSO4 8.201e-005 8.220e-005 -4.086 -4.085 0.001

CaCO3 5.626e-006 5.639e-006 -5.250 -5.249 0.001

CaOH+ 4.218e-009 3.812e-009 -8.375 -8.419 -0.044

CaHSO4+ 3.131e-011 2.829e-011 -10.504 -10.548 -0.044

Cl 1.033e-004

Cl- 1.033e-004 9.317e-005 -3.986 -4.031 -0.045

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -42.845 -42.844 0.001

K 2.636e-005

K+ 2.631e-005 2.373e-005 -4.580 -4.625 -0.045

KSO4- 4.463e-008 4.033e-008 -7.350 -7.394 -0.044

KOH 1.225e-012 1.228e-012 -11.912 -11.911 0.001

Li 3.605e-006

Li+ 3.600e-006 3.269e-006 -5.444 -5.486 -0.042

LiSO4- 4.750e-009 4.293e-009 -8.323 -8.367 -0.044

LiOH 1.115e-012 1.117e-012 -11.953 -11.952 0.001

Mg 8.231e-004

Mg+2 7.635e-004 5.189e-004 -3.117 -3.285 -0.168

MgHCO3+ 3.208e-005 2.899e-005 -4.494 -4.538 -0.044

MgSO4 2.646e-005 2.652e-005 -4.577 -4.576 0.001

MgCO3 1.075e-006 1.078e-006 -5.969 -5.967 0.001

MgOH+ 1.006e-008 9.089e-009 -7.997 -8.041 -0.044

N(5) 2.393e-005

NO3- 2.393e-005 2.155e-005 -4.621 -4.667 -0.046

Na 3.116e-004

Na+ 3.104e-004 2.808e-004 -3.508 -3.552 -0.044

NaHCO3 7.811e-007 7.829e-007 -6.107 -6.106 0.001

NaSO4- 4.328e-007 3.911e-007 -6.364 -6.408 -0.044

NaCO3- 8.059e-009 7.283e-009 -8.094 -8.138 -0.044

NaOH 2.762e-011 2.768e-011 -10.559 -10.558 0.001

O(0) 3.733e-011

O2 1.866e-011 1.871e-011 -10.729 -10.728 0.001

S(6) 5.568e-004

SO4-2 4.475e-004 3.008e-004 -3.349 -3.522 -0.172

CaSO4 8.201e-005 8.220e-005 -4.086 -4.085 0.001

MgSO4 2.646e-005 2.652e-005 -4.577 -4.576 0.001

NaSO4- 4.328e-007 3.911e-007 -6.364 -6.408 -0.044

SrSO4 3.166e-007 3.173e-007 -6.500 -6.499 0.001

BaSO4 6.219e-008 6.234e-008 -7.206 -7.205 0.001

KSO4- 4.463e-008 4.033e-008 -7.350 -7.394 -0.044

LiSO4- 4.750e-009 4.293e-009 -8.323 -8.367 -0.044

HSO4- 1.692e-009 1.529e-009 -8.772 -8.816 -0.044

CaHSO4+ 3.131e-011 2.829e-011 -10.504 -10.548 -0.044

Si 9.492e-005

H4SiO4 9.477e-005 9.499e-005 -4.023 -4.022 0.001

H3SiO4- 1.472e-007 1.330e-007 -6.832 -6.876 -0.044

H2SiO4-2 8.744e-014 5.831e-014 -13.058 -13.234 -0.176

Sr 9.935e-006

Sr+2 9.263e-006 6.268e-006 -5.033 -5.203 -0.170

SrHCO3+ 3.477e-007 3.152e-007 -6.459 -6.501 -0.043

SrSO4 3.166e-007 3.173e-007 -6.500 -6.499 0.001

SrCO3 7.329e-009 7.346e-009 -8.135 -8.134 0.001

SrOH+ 5.296e-012 4.796e-012 -11.276 -11.319 -0.043

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.00 -6.33 -4.33 CaSO4

Aragonite -0.13 -8.39 -8.27 CaCO3

Barite 0.28 -9.91 -10.18 BaSO4

Calcite 0.03 -8.39 -8.42 CaCO3

Celestite -2.10 -8.72 -6.62 SrSO4

Chalcedony -0.33 -4.02 -3.70 SiO2

Chrysotile -8.60 25.14 33.75 Mg3Si2O5(OH)4

CO2(g) -1.73 -3.04 -1.31 CO2

Dolomite -0.46 -17.26 -16.80 CaMg(CO3)2

Gypsum -1.75 -6.33 -4.59 CaSO4:2H2O

H2(g) -39.75 -42.84 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.14 -7.58 1.55 NaCl

O2(g) -7.93 -10.73 -2.79 O2

Quartz 0.14 -4.02 -4.16 SiO2

Sepiolite -6.03 10.06 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.60 10.06 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.21 -4.02 -2.81 SiO2

Strontianite -1.51 -10.79 -9.28 SrCO3

Talc -5.72 17.10 22.82 Mg3Si4O10(OH)2

Witherite -3.36 -11.97 -8.61 BaCO3

Initial solution 5. 06-9-24

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 6.510e-003 6.510e-003

B 3.332e-006 3.332e-006

Ba 6.775e-007 6.775e-007

Ca 2.606e-003 2.606e-003

Cl 8.410e-005 8.410e-005

K 2.482e-005 2.482e-005

Li 3.605e-006 3.605e-006

Mg 9.095e-004 9.095e-004

N(5) 1.857e-006 1.857e-006

Na 3.251e-004 3.251e-004

S(6) 3.862e-004 3.862e-004

Si 9.326e-005 9.326e-005

Sr 1.142e-005 1.142e-005

----------------------------Description of solution----------------------------

pH = 7.032 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 487

Density (g/cm3) = 0.99986

Activity of water = 1.000

Ionic strength = 1.068e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.952e-003

Total CO2 (mol/kg) = 7.952e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = 4.110e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.29

Iterations = 9

Total H = 1.110193e+002

Total O = 5.553055e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

H+ 1.019e-007 9.297e-008 -6.992 -7.032 -0.040

OH- 4.548e-008 4.089e-008 -7.342 -7.388 -0.046

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 3.332e-006

H3BO3 3.314e-006 3.322e-006 -5.480 -5.479 0.001

H2BO3- 1.816e-008 1.637e-008 -7.741 -7.786 -0.045

Ba 6.775e-007

Ba+2 6.180e-007 4.114e-007 -6.209 -6.386 -0.177

BaSO4 4.198e-008 4.208e-008 -7.377 -7.376 0.001

BaHCO3+ 1.721e-008 1.551e-008 -7.764 -7.809 -0.045

BaCO3 3.636e-010 3.645e-010 -9.439 -9.438 0.001

BaOH+ 1.663e-013 1.499e-013 -12.779 -12.824 -0.045

C(4) 7.952e-003

HCO3- 6.345e-003 5.738e-003 -2.198 -2.241 -0.044

CO2 1.451e-003 1.455e-003 -2.838 -2.837 0.001

CaHCO3+ 1.040e-004 9.408e-005 -3.983 -4.026 -0.044

MgHCO3+ 4.093e-005 3.688e-005 -4.388 -4.433 -0.045

CaCO3 4.967e-006 4.980e-006 -5.304 -5.303 0.001

CO3-2 3.264e-006 2.183e-006 -5.486 -5.661 -0.175

MgCO3 9.858e-007 9.882e-007 -6.006 -6.005 0.001

NaHCO3 9.405e-007 9.428e-007 -6.027 -6.026 0.001

SrHCO3+ 4.614e-007 4.173e-007 -6.336 -6.380 -0.044

BaHCO3+ 1.721e-008 1.551e-008 -7.764 -7.809 -0.045

NaCO3- 7.014e-009 6.321e-009 -8.154 -8.199 -0.045

SrCO3 6.991e-009 7.009e-009 -8.155 -8.154 0.001

BaCO3 3.636e-010 3.645e-010 -9.439 -9.438 0.001

Ca 2.606e-003

Ca+2 2.438e-003 1.630e-003 -2.613 -2.788 -0.175

CaHCO3+ 1.040e-004 9.408e-005 -3.983 -4.026 -0.044

CaSO4 5.891e-005 5.906e-005 -4.230 -4.229 0.001

CaCO3 4.967e-006 4.980e-006 -5.304 -5.303 0.001

CaOH+ 3.228e-009 2.908e-009 -8.491 -8.536 -0.045

CaHSO4+ 3.130e-011 2.820e-011 -10.505 -10.550 -0.045

Cl 8.410e-005

Cl- 8.410e-005 7.565e-005 -4.075 -4.121 -0.046

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -42.560 -42.559 0.001

K 2.482e-005

K+ 2.479e-005 2.230e-005 -4.606 -4.652 -0.046

KSO4- 2.853e-008 2.571e-008 -7.545 -7.590 -0.045

KOH 8.294e-013 8.315e-013 -12.081 -12.080 0.001

Li 3.605e-006

Li+ 3.602e-006 3.263e-006 -5.443 -5.486 -0.043

LiSO4- 3.226e-009 2.907e-009 -8.491 -8.537 -0.045

LiOH 8.018e-013 8.037e-013 -12.096 -12.095 0.001

Mg 9.095e-004

Mg+2 8.479e-004 5.705e-004 -3.072 -3.244 -0.172

MgHCO3+ 4.093e-005 3.688e-005 -4.388 -4.433 -0.045

MgSO4 1.973e-005 1.978e-005 -4.705 -4.704 0.001

MgCO3 9.858e-007 9.882e-007 -6.006 -6.005 0.001

MgOH+ 7.992e-009 7.202e-009 -8.097 -8.143 -0.045

N(5) 1.857e-006

NO3- 1.857e-006 1.667e-006 -5.731 -5.778 -0.047

Na 3.251e-004

Na+ 3.239e-004 2.922e-004 -3.490 -3.534 -0.045

NaHCO3 9.405e-007 9.428e-007 -6.027 -6.026 0.001

NaSO4- 3.064e-007 2.761e-007 -6.514 -6.559 -0.045

NaCO3- 7.014e-009 6.321e-009 -8.154 -8.199 -0.045

NaOH 2.071e-011 2.076e-011 -10.684 -10.683 0.001

O(0) 1.007e-011

O2 5.036e-012 5.048e-012 -11.298 -11.297 0.001

S(6) 3.862e-004

SO4-2 3.069e-004 2.041e-004 -3.513 -3.690 -0.177

CaSO4 5.891e-005 5.906e-005 -4.230 -4.229 0.001

MgSO4 1.973e-005 1.978e-005 -4.705 -4.704 0.001

NaSO4- 3.064e-007 2.761e-007 -6.514 -6.559 -0.045

SrSO4 2.457e-007 2.463e-007 -6.610 -6.609 0.001

BaSO4 4.198e-008 4.208e-008 -7.377 -7.376 0.001

KSO4- 2.853e-008 2.571e-008 -7.545 -7.590 -0.045

LiSO4- 3.226e-009 2.907e-009 -8.491 -8.537 -0.045

HSO4- 1.597e-009 1.439e-009 -8.797 -8.842 -0.045

CaHSO4+ 3.130e-011 2.820e-011 -10.505 -10.550 -0.045

Si 9.326e-005

H4SiO4 9.315e-005 9.338e-005 -4.031 -4.030 0.001

H3SiO4- 1.046e-007 9.424e-008 -6.981 -7.026 -0.045

H2SiO4-2 4.515e-014 2.978e-014 -13.345 -13.526 -0.181

Sr 1.142e-005

Sr+2 1.071e-005 7.169e-006 -4.970 -5.145 -0.174

SrHCO3+ 4.614e-007 4.173e-007 -6.336 -6.380 -0.044

SrSO4 2.457e-007 2.463e-007 -6.610 -6.609 0.001

SrCO3 6.991e-009 7.009e-009 -8.155 -8.154 0.001

SrOH+ 4.377e-012 3.954e-012 -11.359 -11.403 -0.044

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.14 -6.48 -4.33 CaSO4

Aragonite -0.18 -8.45 -8.27 CaCO3

Barite 0.11 -10.08 -10.18 BaSO4

Calcite -0.03 -8.45 -8.42 CaCO3

Celestite -2.21 -8.83 -6.62 SrSO4

Chalcedony -0.33 -4.03 -3.70 SiO2

Chrysotile -9.35 24.40 33.75 Mg3Si2O5(OH)4

CO2(g) -1.52 -2.84 -1.31 CO2

Dolomite -0.55 -17.35 -16.80 CaMg(CO3)2

Gypsum -1.89 -6.48 -4.59 CaSO4:2H2O

H2(g) -39.46 -42.56 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.21 -7.66 1.55 NaCl

O2(g) -8.50 -11.30 -2.79 O2

Quartz 0.13 -4.03 -4.16 SiO2

Sepiolite -6.54 9.55 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -9.11 9.55 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.21 -4.03 -2.81 SiO2

Strontianite -1.53 -10.81 -9.28 SrCO3

Talc -6.48 16.34 22.82 Mg3Si4O10(OH)2

Witherite -3.44 -12.05 -8.61 BaCO3

Initial solution 6. 06-10-12

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 2.596e-007 2.596e-007

Alkalinity 6.625e-003 6.625e-003

B 3.147e-006 3.147e-006

Ba 7.723e-007 7.723e-007

Ca 2.604e-003 2.604e-003

Cl 9.088e-005 9.088e-005

K 2.329e-005 2.329e-005

Li 3.605e-006 3.605e-006

Mg 8.807e-004 8.807e-004

N(5) 1.286e-006 1.286e-006

Na 3.168e-004 3.168e-004

S(6) 3.622e-004 3.622e-004

Si 9.326e-005 9.326e-005

Sr 1.028e-005 1.028e-005

----------------------------Description of solution----------------------------

pH = 7.036 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 487

Density (g/cm3) = 0.99986

Activity of water = 1.000

Ionic strength = 1.064e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 8.077e-003

Total CO2 (mol/kg) = 8.077e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -1.055e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.75

Iterations = 11

Total H = 1.110194e+002

Total O = 5.553082e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

H+ 1.009e-007 9.207e-008 -6.996 -7.036 -0.040

OH- 4.591e-008 4.129e-008 -7.338 -7.384 -0.046

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 2.596e-007

Al(OH)4- 2.269e-007 2.045e-007 -6.644 -6.689 -0.045

Al(OH)2+ 2.039e-008 1.838e-008 -7.691 -7.736 -0.045

Al(OH)3 1.124e-008 1.127e-008 -7.949 -7.948 0.001

AlOH+2 1.009e-009 6.660e-010 -8.996 -9.177 -0.181

Al+3 3.123e-011 1.376e-011 -10.505 -10.861 -0.356

AlSO4+ 7.873e-012 7.096e-012 -11.104 -11.149 -0.045

Al(SO4)2- 4.506e-014 4.061e-014 -13.346 -13.391 -0.045

AlHSO4+2 8.054e-020 5.315e-020 -19.094 -19.275 -0.181

B 3.147e-006

H3BO3 3.130e-006 3.137e-006 -5.504 -5.503 0.001

H2BO3- 1.732e-008 1.561e-008 -7.762 -7.807 -0.045

Ba 7.723e-007

Ba+2 7.067e-007 4.707e-007 -6.151 -6.327 -0.176

BaSO4 4.514e-008 4.525e-008 -7.345 -7.344 0.001

BaHCO3+ 2.004e-008 1.806e-008 -7.698 -7.743 -0.045

BaCO3 4.276e-010 4.287e-010 -9.369 -9.368 0.001

BaOH+ 1.922e-013 1.732e-013 -12.716 -12.761 -0.045

C(4) 8.077e-003

HCO3- 6.457e-003 5.840e-003 -2.190 -2.234 -0.044

CO2 1.463e-003 1.467e-003 -2.835 -2.834 0.001

CaHCO3+ 1.059e-004 9.578e-005 -3.975 -4.019 -0.044

MgHCO3+ 4.037e-005 3.639e-005 -4.394 -4.439 -0.045

CaCO3 5.107e-006 5.119e-006 -5.292 -5.291 0.001

CO3-2 3.352e-006 2.243e-006 -5.475 -5.649 -0.174

MgCO3 9.821e-007 9.846e-007 -6.008 -6.007 0.001

NaHCO3 9.330e-007 9.353e-007 -6.030 -6.029 0.001

SrHCO3+ 4.231e-007 3.827e-007 -6.374 -6.417 -0.044

BaHCO3+ 2.004e-008 1.806e-008 -7.698 -7.743 -0.045

NaCO3- 7.026e-009 6.332e-009 -8.153 -8.198 -0.045

SrCO3 6.474e-009 6.490e-009 -8.189 -8.188 0.001

BaCO3 4.276e-010 4.287e-010 -9.369 -9.368 0.001

Ca 2.604e-003

Ca+2 2.437e-003 1.630e-003 -2.613 -2.788 -0.175

CaHCO3+ 1.059e-004 9.578e-005 -3.975 -4.019 -0.044

CaSO4 5.537e-005 5.551e-005 -4.257 -4.256 0.001

CaCO3 5.107e-006 5.119e-006 -5.292 -5.291 0.001

CaOH+ 3.259e-009 2.938e-009 -8.487 -8.532 -0.045

CaHSO4+ 2.913e-011 2.625e-011 -10.536 -10.581 -0.045

Cl 9.088e-005

Cl- 9.088e-005 8.175e-005 -4.042 -4.087 -0.046

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -42.569 -42.568 0.001

K 2.329e-005

K+ 2.326e-005 2.093e-005 -4.633 -4.679 -0.046

KSO4- 2.516e-008 2.267e-008 -7.599 -7.644 -0.045

KOH 7.859e-013 7.879e-013 -12.105 -12.104 0.001

Li 3.605e-006

Li+ 3.602e-006 3.263e-006 -5.443 -5.486 -0.043

LiSO4- 3.031e-009 2.732e-009 -8.518 -8.563 -0.045

LiOH 8.098e-013 8.117e-013 -12.092 -12.091 0.001

Mg 8.807e-004

Mg+2 8.214e-004 5.530e-004 -3.085 -3.257 -0.172

MgHCO3+ 4.037e-005 3.639e-005 -4.394 -4.439 -0.045

MgSO4 1.797e-005 1.802e-005 -4.745 -4.744 0.001

MgCO3 9.821e-007 9.846e-007 -6.008 -6.007 0.001

MgOH+ 7.821e-009 7.049e-009 -8.107 -8.152 -0.045

N(5) 1.286e-006

NO3- 1.286e-006 1.154e-006 -5.891 -5.938 -0.047

Na 3.168e-004

Na+ 3.156e-004 2.848e-004 -3.501 -3.545 -0.045

NaHCO3 9.330e-007 9.353e-007 -6.030 -6.029 0.001

NaSO4- 2.806e-007 2.529e-007 -6.552 -6.597 -0.045

NaCO3- 7.026e-009 6.332e-009 -8.153 -8.198 -0.045

NaOH 2.038e-011 2.043e-011 -10.691 -10.690 0.001

O(0) 1.047e-011

O2 5.236e-012 5.248e-012 -11.281 -11.280 0.001

S(6) 3.622e-004

SO4-2 2.882e-004 1.918e-004 -3.540 -3.717 -0.177

CaSO4 5.537e-005 5.551e-005 -4.257 -4.256 0.001

MgSO4 1.797e-005 1.802e-005 -4.745 -4.744 0.001

NaSO4- 2.806e-007 2.529e-007 -6.552 -6.597 -0.045

SrSO4 2.080e-007 2.085e-007 -6.682 -6.681 0.001

BaSO4 4.514e-008 4.525e-008 -7.345 -7.344 0.001

KSO4- 2.516e-008 2.267e-008 -7.599 -7.644 -0.045

LiSO4- 3.031e-009 2.732e-009 -8.518 -8.563 -0.045

HSO4- 1.486e-009 1.339e-009 -8.828 -8.873 -0.045

CaHSO4+ 2.913e-011 2.625e-011 -10.536 -10.581 -0.045

AlSO4+ 7.873e-012 7.096e-012 -11.104 -11.149 -0.045

Al(SO4)2- 4.506e-014 4.061e-014 -13.346 -13.391 -0.045

AlHSO4+2 8.054e-020 5.315e-020 -19.094 -19.275 -0.181

Si 9.326e-005

H4SiO4 9.315e-005 9.338e-005 -4.031 -4.030 0.001

H3SiO4- 1.056e-007 9.516e-008 -6.976 -7.022 -0.045

H2SiO4-2 4.601e-014 3.036e-014 -13.337 -13.518 -0.181

Sr 1.028e-005

Sr+2 9.640e-006 6.460e-006 -5.016 -5.190 -0.174

SrHCO3+ 4.231e-007 3.827e-007 -6.374 -6.417 -0.044

SrSO4 2.080e-007 2.085e-007 -6.682 -6.681 0.001

SrCO3 6.474e-009 6.490e-009 -8.189 -8.188 0.001

SrOH+ 3.982e-012 3.597e-012 -11.400 -11.444 -0.044

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -1.37 10.25 11.61 Al(OH)3

Albite -3.53 -22.32 -18.80 NaAlSi3O8

Alunite -2.63 -2.48 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.17 -6.50 -4.33 CaSO4

Anorthite -4.16 -24.23 -20.07 CaAl2Si2O8

Aragonite -0.17 -8.44 -8.27 CaCO3

Barite 0.14 -10.04 -10.18 BaSO4

Ca-Montmorillonite 1.92 -44.91 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite -0.02 -8.44 -8.42 CaCO3

Celestite -2.28 -8.91 -6.62 SrSO4

Chalcedony -0.33 -4.03 -3.70 SiO2

Chlorite(14A) -10.56 62.47 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -9.36 24.38 33.75 Mg3Si2O5(OH)4

CO2(g) -1.52 -2.83 -1.31 CO2

Dolomite -0.54 -17.34 -16.80 CaMg(CO3)2

Gibbsite 1.44 10.25 8.81 Al(OH)3

Gypsum -1.92 -6.51 -4.59 CaSO4:2H2O

H2(g) -39.47 -42.57 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.19 -7.63 1.55 NaCl

Illite 0.39 -41.55 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -1.94 -23.46 -21.52 KAlSi3O8

K-mica 6.48 21.01 14.53 KAl3Si3O10(OH)2

Kaolinite 3.91 12.43 8.52 Al2Si2O5(OH)4

O2(g) -8.49 -11.28 -2.79 O2

Quartz 0.13 -4.03 -4.16 SiO2

Sepiolite -6.55 9.54 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -9.12 9.54 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.21 -4.03 -2.81 SiO2

Strontianite -1.56 -10.84 -9.28 SrCO3

Talc -6.50 16.32 22.82 Mg3Si4O10(OH)2

Witherite -3.37 -11.98 -8.61 BaCO3

Initial solution 7. 06-11-18

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 6.543e-003 6.543e-003

B 2.684e-006 2.684e-006

Ba 6.047e-007 6.047e-007

Ca 2.534e-003 2.534e-003

Cl 1.106e-004 1.106e-004

K 1.894e-005 1.894e-005

Li 3.605e-006 3.605e-006

Mg 9.260e-004 9.260e-004

Na 3.212e-004 3.212e-004

S(6) 4.416e-004 4.416e-004

Si 8.660e-005 8.660e-005

Sr 1.153e-005 1.153e-005

----------------------------Description of solution----------------------------

pH = 7.133 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 488

Density (g/cm3) = 0.99986

Activity of water = 1.000

Ionic strength = 1.066e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.685e-003

Total CO2 (mol/kg) = 7.685e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -2.488e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.76

Iterations = 9

Total H = 1.110193e+002

Total O = 5.553024e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

H+ 8.057e-008 7.355e-008 -7.094 -7.133 -0.040

OH- 5.749e-008 5.169e-008 -7.240 -7.287 -0.046

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 2.684e-006

H3BO3 2.666e-006 2.672e-006 -5.574 -5.573 0.001

H2BO3- 1.847e-008 1.664e-008 -7.734 -7.779 -0.045

Ba 6.047e-007

Ba+2 5.464e-007 3.638e-007 -6.263 -6.439 -0.177

BaSO4 4.264e-008 4.274e-008 -7.370 -7.369 0.001

BaHCO3+ 1.529e-008 1.378e-008 -7.816 -7.861 -0.045

BaCO3 4.085e-010 4.095e-010 -9.389 -9.388 0.001

BaOH+ 1.859e-013 1.676e-013 -12.731 -12.776 -0.045

C(4) 7.685e-003

HCO3- 6.375e-003 5.766e-003 -2.196 -2.239 -0.044

CO2 1.154e-003 1.156e-003 -2.938 -2.937 0.001

CaHCO3+ 1.012e-004 9.156e-005 -3.995 -4.038 -0.044

MgHCO3+ 4.172e-005 3.760e-005 -4.380 -4.425 -0.045

CaCO3 6.111e-006 6.126e-006 -5.214 -5.213 0.001

CO3-2 4.145e-006 2.773e-006 -5.382 -5.557 -0.175

MgCO3 1.270e-006 1.274e-006 -5.896 -5.895 0.001

NaHCO3 9.335e-007 9.358e-007 -6.030 -6.029 0.001

SrHCO3+ 4.667e-007 4.221e-007 -6.331 -6.375 -0.044

BaHCO3+ 1.529e-008 1.378e-008 -7.816 -7.861 -0.045

SrCO3 8.940e-009 8.962e-009 -8.049 -8.048 0.001

NaCO3- 8.801e-009 7.932e-009 -8.055 -8.101 -0.045

BaCO3 4.085e-010 4.095e-010 -9.389 -9.388 0.001

Ca 2.534e-003

Ca+2 2.361e-003 1.578e-003 -2.627 -2.802 -0.175

CaHCO3+ 1.012e-004 9.156e-005 -3.995 -4.038 -0.044

CaSO4 6.553e-005 6.569e-005 -4.184 -4.183 0.001

CaCO3 6.111e-006 6.126e-006 -5.214 -5.213 0.001

CaOH+ 3.951e-009 3.561e-009 -8.403 -8.448 -0.045

CaHSO4+ 2.753e-011 2.481e-011 -10.560 -10.605 -0.045

Cl 1.106e-004

Cl- 1.106e-004 9.952e-005 -3.956 -4.002 -0.046

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -42.764 -42.763 0.001

K 1.894e-005

K+ 1.891e-005 1.701e-005 -4.723 -4.769 -0.046

KSO4- 2.500e-008 2.253e-008 -7.602 -7.647 -0.045

KOH 7.998e-013 8.018e-013 -12.097 -12.096 0.001

Li 3.605e-006

Li+ 3.601e-006 3.262e-006 -5.444 -5.486 -0.043

LiSO4- 3.704e-009 3.338e-009 -8.431 -8.476 -0.045

LiOH 1.013e-012 1.016e-012 -11.994 -11.993 0.001

Mg 9.260e-004

Mg+2 8.600e-004 5.788e-004 -3.065 -3.237 -0.172

MgHCO3+ 4.172e-005 3.760e-005 -4.380 -4.425 -0.045

MgSO4 2.299e-005 2.305e-005 -4.638 -4.637 0.001

MgCO3 1.270e-006 1.274e-006 -5.896 -5.895 0.001

MgOH+ 1.025e-008 9.237e-009 -7.989 -8.034 -0.045

Na 3.212e-004

Na+ 3.199e-004 2.886e-004 -3.495 -3.540 -0.045

NaHCO3 9.335e-007 9.358e-007 -6.030 -6.029 0.001

NaSO4- 3.476e-007 3.133e-007 -6.459 -6.504 -0.045

NaCO3- 8.801e-009 7.932e-009 -8.055 -8.101 -0.045

NaOH 2.586e-011 2.592e-011 -10.587 -10.586 0.001

O(0) 2.572e-011

O2 1.286e-011 1.289e-011 -10.891 -10.890 0.001

S(6) 4.416e-004

SO4-2 3.524e-004 2.344e-004 -3.453 -3.630 -0.177

CaSO4 6.553e-005 6.569e-005 -4.184 -4.183 0.001

MgSO4 2.299e-005 2.305e-005 -4.638 -4.637 0.001

NaSO4- 3.476e-007 3.133e-007 -6.459 -6.504 -0.045

SrSO4 2.840e-007 2.847e-007 -6.547 -6.546 0.001

BaSO4 4.264e-008 4.274e-008 -7.370 -7.369 0.001

KSO4- 2.500e-008 2.253e-008 -7.602 -7.647 -0.045

LiSO4- 3.704e-009 3.338e-009 -8.431 -8.476 -0.045

HSO4- 1.451e-009 1.308e-009 -8.838 -8.884 -0.045

CaHSO4+ 2.753e-011 2.481e-011 -10.560 -10.605 -0.045

Si 8.660e-005

H4SiO4 8.647e-005 8.669e-005 -4.063 -4.062 0.001

H3SiO4- 1.227e-007 1.106e-007 -6.911 -6.956 -0.045

H2SiO4-2 6.697e-014 4.418e-014 -13.174 -13.355 -0.181

Sr 1.153e-005

Sr+2 1.077e-005 7.217e-006 -4.968 -5.142 -0.174

SrHCO3+ 4.667e-007 4.221e-007 -6.331 -6.375 -0.044

SrSO4 2.840e-007 2.847e-007 -6.547 -6.546 0.001

SrCO3 8.940e-009 8.962e-009 -8.049 -8.048 0.001

SrOH+ 5.570e-012 5.032e-012 -11.254 -11.298 -0.044

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.10 -6.43 -4.33 CaSO4

Aragonite -0.09 -8.36 -8.27 CaCO3

Barite 0.11 -10.07 -10.18 BaSO4

Calcite 0.06 -8.36 -8.42 CaCO3

Celestite -2.15 -8.77 -6.62 SrSO4

Chalcedony -0.37 -4.06 -3.70 SiO2

Chrysotile -8.78 24.96 33.75 Mg3Si2O5(OH)4

CO2(g) -1.62 -2.94 -1.31 CO2

Dolomite -0.35 -17.15 -16.80 CaMg(CO3)2

Gypsum -1.85 -6.43 -4.59 CaSO4:2H2O

H2(g) -39.67 -42.76 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.10 -7.54 1.55 NaCl

O2(g) -8.10 -10.89 -2.79 O2

Quartz 0.10 -4.06 -4.16 SiO2

Sepiolite -6.22 9.87 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.79 9.87 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.25 -4.06 -2.81 SiO2

Strontianite -1.42 -10.70 -9.28 SrCO3

Talc -5.98 16.84 22.82 Mg3Si4O10(OH)2

Witherite -3.39 -12.00 -8.61 BaCO3

Initial solution 8. 07-1-4

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 6.444e-003 6.444e-003

B 2.129e-006 2.129e-006

Ba 7.504e-007 7.504e-007

Ca 2.669e-003 2.669e-003

Cl 8.608e-005 8.608e-005

K 1.663e-005 1.663e-005

Li 3.317e-006 3.317e-006

Mg 9.054e-004 9.054e-004

Na 3.182e-004 3.182e-004

S(6) 4.913e-004 4.913e-004

Si 8.160e-005 8.160e-005

Sr 1.039e-005 1.039e-005

----------------------------Description of solution----------------------------

pH = 7.284 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 494

Density (g/cm3) = 0.99987

Activity of water = 1.000

Ionic strength = 1.087e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.228e-003

Total CO2 (mol/kg) = 7.228e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -4.378e-006

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.03

Iterations = 9

Total H = 1.110192e+002

Total O = 5.552940e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.145e-008 7.317e-008 -7.089 -7.136 -0.047

H+ 5.695e-008 5.196e-008 -7.244 -7.284 -0.040

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 2.129e-006

H3BO3 2.108e-006 2.113e-006 -5.676 -5.675 0.001

H2BO3- 2.069e-008 1.863e-008 -7.684 -7.730 -0.046

Ba 7.504e-007

Ba+2 6.734e-007 4.469e-007 -6.172 -6.350 -0.178

BaSO4 5.780e-008 5.794e-008 -7.238 -7.237 0.001

BaHCO3+ 1.846e-008 1.663e-008 -7.734 -7.779 -0.046

BaCO3 6.976e-010 6.994e-010 -9.156 -9.155 0.001

BaOH+ 3.236e-013 2.914e-013 -12.490 -12.535 -0.046

C(4) 7.228e-003

HCO3- 6.266e-003 5.662e-003 -2.203 -2.247 -0.044

CO2 8.003e-004 8.024e-004 -3.097 -3.096 0.001

CaHCO3+ 1.042e-004 9.414e-005 -3.982 -4.026 -0.044

MgHCO3+ 3.989e-005 3.592e-005 -4.399 -4.445 -0.046

CaCO3 8.894e-006 8.916e-006 -5.051 -5.050 0.001

CO3-2 5.780e-006 3.854e-006 -5.238 -5.414 -0.176

MgCO3 1.718e-006 1.722e-006 -5.765 -5.764 0.001

NaHCO3 9.072e-007 9.095e-007 -6.042 -6.041 0.001

SrHCO3+ 4.112e-007 3.716e-007 -6.386 -6.430 -0.044

BaHCO3+ 1.846e-008 1.663e-008 -7.734 -7.779 -0.046

NaCO3- 1.212e-008 1.091e-008 -7.917 -7.962 -0.046

SrCO3 1.114e-008 1.117e-008 -7.953 -7.952 0.001

BaCO3 6.976e-010 6.994e-010 -9.156 -9.155 0.001

Ca 2.669e-003

Ca+2 2.480e-003 1.653e-003 -2.606 -2.782 -0.176

CaHCO3+ 1.042e-004 9.414e-005 -3.982 -4.026 -0.044

CaSO4 7.571e-005 7.590e-005 -4.121 -4.120 0.001

CaCO3 8.894e-006 8.916e-006 -5.051 -5.050 0.001

CaOH+ 5.861e-009 5.278e-009 -8.232 -8.278 -0.046

CaHSO4+ 2.249e-011 2.025e-011 -10.648 -10.693 -0.046

Cl 8.608e-005

Cl- 8.608e-005 7.736e-005 -4.065 -4.111 -0.046

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.066 -43.065 0.001

K 1.663e-005

K+ 1.661e-005 1.493e-005 -4.780 -4.826 -0.046

KSO4- 2.422e-008 2.181e-008 -7.616 -7.661 -0.046

KOH 9.934e-013 9.959e-013 -12.003 -12.002 0.001

Li 3.317e-006

Li+ 3.313e-006 2.999e-006 -5.480 -5.523 -0.043

LiSO4- 3.761e-009 3.386e-009 -8.425 -8.470 -0.046

LiOH 1.319e-012 1.322e-012 -11.880 -11.879 0.001

Mg 9.054e-004

Mg+2 8.391e-004 5.630e-004 -3.076 -3.250 -0.173

MgHCO3+ 3.989e-005 3.592e-005 -4.399 -4.445 -0.046

MgSO4 2.468e-005 2.474e-005 -4.608 -4.607 0.001

MgCO3 1.718e-006 1.722e-006 -5.765 -5.764 0.001

MgOH+ 1.412e-008 1.272e-008 -7.850 -7.896 -0.046

Na 3.182e-004

Na+ 3.169e-004 2.856e-004 -3.499 -3.544 -0.045

NaHCO3 9.072e-007 9.095e-007 -6.042 -6.041 0.001

NaSO4- 3.799e-007 3.421e-007 -6.420 -6.466 -0.046

NaCO3- 1.212e-008 1.091e-008 -7.917 -7.962 -0.046

NaOH 3.623e-011 3.632e-011 -10.441 -10.440 0.001

O(0) 1.033e-010

O2 5.163e-011 5.176e-011 -10.287 -10.286 0.001

S(6) 4.913e-004

SO4-2 3.902e-004 2.587e-004 -3.409 -3.587 -0.178

CaSO4 7.571e-005 7.590e-005 -4.121 -4.120 0.001

MgSO4 2.468e-005 2.474e-005 -4.608 -4.607 0.001

NaSO4- 3.799e-007 3.421e-007 -6.420 -6.466 -0.046

SrSO4 2.809e-007 2.816e-007 -6.551 -6.550 0.001

BaSO4 5.780e-008 5.794e-008 -7.238 -7.237 0.001

KSO4- 2.422e-008 2.181e-008 -7.616 -7.661 -0.046

LiSO4- 3.761e-009 3.386e-009 -8.425 -8.470 -0.046

HSO4- 1.132e-009 1.019e-009 -8.946 -8.992 -0.046

CaHSO4+ 2.249e-011 2.025e-011 -10.648 -10.693 -0.046

Si 8.160e-005

H4SiO4 8.144e-005 8.164e-005 -4.089 -4.088 0.001

H3SiO4- 1.637e-007 1.474e-007 -6.786 -6.831 -0.046

H2SiO4-2 1.268e-013 8.336e-014 -12.897 -13.079 -0.182

Sr 1.039e-005

Sr+2 9.689e-006 6.469e-006 -5.014 -5.189 -0.175

SrHCO3+ 4.112e-007 3.716e-007 -6.386 -6.430 -0.044

SrSO4 2.809e-007 2.816e-007 -6.551 -6.550 0.001

SrCO3 1.114e-008 1.117e-008 -7.953 -7.952 0.001

SrOH+ 7.074e-012 6.384e-012 -11.150 -11.195 -0.045

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.03 -6.37 -4.33 CaSO4

Aragonite 0.07 -8.20 -8.27 CaCO3

Barite 0.25 -9.94 -10.18 BaSO4

Calcite 0.23 -8.20 -8.42 CaCO3

Celestite -2.15 -8.78 -6.62 SrSO4

Chalcedony -0.39 -4.09 -3.70 SiO2

Chrysotile -7.97 25.78 33.75 Mg3Si2O5(OH)4

CO2(g) -1.78 -3.10 -1.31 CO2

Dolomite -0.06 -16.86 -16.80 CaMg(CO3)2

Gypsum -1.78 -6.37 -4.59 CaSO4:2H2O

H2(g) -39.97 -43.06 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.21 -7.66 1.55 NaCl

O2(g) -7.49 -10.29 -2.79 O2

Quartz 0.08 -4.09 -4.16 SiO2

Sepiolite -5.71 10.37 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.29 10.37 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.27 -4.09 -2.81 SiO2

Strontianite -1.32 -10.60 -9.28 SrCO3

Talc -5.22 17.61 22.82 Mg3Si4O10(OH)2

Witherite -3.15 -11.76 -8.61 BaCO3

Initial solution 9. 07-2-18

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 5.783e-003 5.783e-003

B 1.759e-006 1.759e-006

Ba 6.047e-007 6.047e-007

Ca 2.347e-003 2.347e-003

Cl 6.830e-005 6.830e-005

K 1.714e-005 1.714e-005

Li 3.172e-006 3.172e-006

Mg 8.148e-004 8.148e-004

Na 2.824e-004 2.824e-004

S(6) 4.601e-004 4.601e-004

Si 6.661e-005 6.661e-005

Sr 9.135e-006 9.135e-006

----------------------------Description of solution----------------------------

pH = 7.854 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 443

Density (g/cm3) = 0.99982

Activity of water = 1.000

Ionic strength = 9.679e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 5.924e-003

Total CO2 (mol/kg) = 5.924e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -1.268e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.00

Iterations = 9

Total H = 1.110184e+002

Total O = 5.552591e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.007e-007 2.716e-007 -6.522 -6.566 -0.044

H+ 1.528e-008 1.400e-008 -7.816 -7.854 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 1.759e-006

H3BO3 1.697e-006 1.701e-006 -5.770 -5.769 0.001

H2BO3- 6.149e-008 5.565e-008 -7.211 -7.255 -0.043

Ba 6.047e-007

Ba+2 5.430e-007 3.676e-007 -6.265 -6.435 -0.169

BaSO4 4.623e-008 4.633e-008 -7.335 -7.334 0.001

BaHCO3+ 1.349e-008 1.221e-008 -7.870 -7.913 -0.043

BaCO3 1.901e-009 1.906e-009 -8.721 -8.720 0.001

BaOH+ 9.830e-013 8.897e-013 -12.007 -12.051 -0.043

C(4) 5.924e-003

HCO3- 5.565e-003 5.054e-003 -2.255 -2.296 -0.042

CO2 1.925e-004 1.929e-004 -3.716 -3.715 0.001

CaHCO3+ 8.263e-005 7.503e-005 -4.083 -4.125 -0.042

MgHCO3+ 3.248e-005 2.939e-005 -4.488 -4.532 -0.043

CaCO3 2.632e-005 2.637e-005 -4.580 -4.579 0.001

CO3-2 1.878e-005 1.277e-005 -4.726 -4.894 -0.168

MgCO3 5.219e-006 5.231e-006 -5.282 -5.281 0.001

NaHCO3 7.229e-007 7.245e-007 -6.141 -6.140 0.001

SrHCO3+ 3.277e-007 2.976e-007 -6.484 -6.526 -0.042

NaCO3- 3.564e-008 3.226e-008 -7.448 -7.491 -0.043

SrCO3 3.313e-008 3.320e-008 -7.480 -7.479 0.001

BaHCO3+ 1.349e-008 1.221e-008 -7.870 -7.913 -0.043

BaCO3 1.901e-009 1.906e-009 -8.721 -8.720 0.001

Ca 2.347e-003

Ca+2 2.172e-003 1.476e-003 -2.663 -2.831 -0.168

CaHCO3+ 8.263e-005 7.503e-005 -4.083 -4.125 -0.042

CaSO4 6.573e-005 6.588e-005 -4.182 -4.181 0.001

CaCO3 2.632e-005 2.637e-005 -4.580 -4.579 0.001

CaOH+ 1.933e-008 1.749e-008 -7.714 -7.757 -0.043

CaHSO4+ 5.233e-012 4.737e-012 -11.281 -11.325 -0.043

Cl 6.830e-005

Cl- 6.830e-005 6.171e-005 -4.166 -4.210 -0.044

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -44.205 -44.204 0.001

K 1.714e-005

K+ 1.712e-005 1.547e-005 -4.767 -4.811 -0.044

KSO4- 2.428e-008 2.197e-008 -7.615 -7.658 -0.043

KOH 3.822e-012 3.831e-012 -11.418 -11.417 0.001

Li 3.172e-006

Li+ 3.169e-006 2.882e-006 -5.499 -5.540 -0.041

LiSO4- 3.495e-009 3.163e-009 -8.457 -8.500 -0.043

LiOH 4.705e-012 4.715e-012 -11.327 -11.327 0.001

Mg 8.148e-004

Mg+2 7.551e-004 5.162e-004 -3.122 -3.287 -0.165

MgHCO3+ 3.248e-005 2.939e-005 -4.488 -4.532 -0.043

MgSO4 2.200e-005 2.205e-005 -4.658 -4.657 0.001

MgCO3 5.219e-006 5.231e-006 -5.282 -5.281 0.001

MgOH+ 4.782e-008 4.328e-008 -7.320 -7.364 -0.043

Na 2.824e-004

Na+ 2.814e-004 2.549e-004 -3.551 -3.594 -0.043

NaHCO3 7.229e-007 7.245e-007 -6.141 -6.140 0.001

NaSO4- 3.279e-007 2.968e-007 -6.484 -6.528 -0.043

NaCO3- 3.564e-008 3.226e-008 -7.448 -7.491 -0.043

NaOH 1.200e-010 1.203e-010 -9.921 -9.920 0.001

O(0) 1.960e-008

O2 9.802e-009 9.824e-009 -8.009 -8.008 0.001

S(6) 4.601e-004

SO4-2 3.718e-004 2.514e-004 -3.430 -3.600 -0.170

CaSO4 6.573e-005 6.588e-005 -4.182 -4.181 0.001

MgSO4 2.200e-005 2.205e-005 -4.658 -4.657 0.001

NaSO4- 3.279e-007 2.968e-007 -6.484 -6.528 -0.043

SrSO4 2.451e-007 2.457e-007 -6.611 -6.610 0.001

BaSO4 4.623e-008 4.633e-008 -7.335 -7.334 0.001

KSO4- 2.428e-008 2.197e-008 -7.615 -7.658 -0.043

LiSO4- 3.495e-009 3.163e-009 -8.457 -8.500 -0.043

HSO4- 2.950e-010 2.670e-010 -9.530 -9.574 -0.043

CaHSO4+ 5.233e-012 4.737e-012 -11.281 -11.325 -0.043

Si 6.661e-005

H4SiO4 6.612e-005 6.626e-005 -4.180 -4.179 0.001

H3SiO4- 4.907e-007 4.441e-007 -6.309 -6.352 -0.043

H2SiO4-2 1.389e-012 9.321e-013 -11.857 -12.031 -0.173

Sr 9.135e-006

Sr+2 8.529e-006 5.806e-006 -5.069 -5.236 -0.167

SrHCO3+ 3.277e-007 2.976e-007 -6.484 -6.526 -0.042

SrSO4 2.451e-007 2.457e-007 -6.611 -6.610 0.001

SrCO3 3.313e-008 3.320e-008 -7.480 -7.479 0.001

SrOH+ 2.345e-011 2.127e-011 -10.630 -10.672 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.10 -6.43 -4.33 CaSO4

Aragonite 0.54 -7.72 -8.27 CaCO3

Barite 0.15 -10.03 -10.18 BaSO4

Calcite 0.70 -7.72 -8.42 CaCO3

Celestite -2.21 -8.84 -6.62 SrSO4

Chalcedony -0.48 -4.18 -3.70 SiO2

Chrysotile -4.84 28.90 33.75 Mg3Si2O5(OH)4

CO2(g) -2.40 -3.71 -1.31 CO2

Dolomite 0.89 -15.91 -16.80 CaMg(CO3)2

Gypsum -1.84 -6.43 -4.59 CaSO4:2H2O

H2(g) -41.11 -44.20 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.36 -7.80 1.55 NaCl

O2(g) -5.21 -8.01 -2.79 O2

Quartz -0.01 -4.18 -4.16 SiO2

Sepiolite -3.78 12.31 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -6.35 12.31 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.36 -4.18 -2.81 SiO2

Strontianite -0.85 -10.13 -9.28 SrCO3

Talc -2.28 20.55 22.82 Mg3Si4O10(OH)2

Witherite -2.72 -11.33 -8.61 BaCO3

Initial solution 10. 07-3-18

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 5.929e-003 5.929e-003

B 1.759e-006 1.759e-006

Ba 6.775e-007 6.775e-007

Ca 2.401e-003 2.401e-003

Cl 7.676e-005 7.676e-005

K 1.510e-005 1.510e-005

Li 2.884e-006 2.884e-006

Mg 8.437e-004 8.437e-004

Na 2.824e-004 2.824e-004

S(6) 3.910e-004 3.910e-004

Si 7.327e-005 7.327e-005

Sr 9.135e-006 9.135e-006

----------------------------Description of solution----------------------------

pH = 7.871 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 448

Density (g/cm3) = 0.99982

Activity of water = 1.000

Ionic strength = 9.812e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.063e-003

Total CO2 (mol/kg) = 6.063e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = 2.241e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.17

Iterations = 9

Total H = 1.110186e+002

Total O = 5.552608e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.127e-007 2.822e-007 -6.505 -6.549 -0.044

H+ 1.471e-008 1.347e-008 -7.832 -7.871 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 1.759e-006

H3BO3 1.695e-006 1.699e-006 -5.771 -5.770 0.001

H2BO3- 6.385e-008 5.776e-008 -7.195 -7.238 -0.044

Ba 6.775e-007

Ba+2 6.155e-007 4.157e-007 -6.211 -6.381 -0.170

BaSO4 4.411e-008 4.420e-008 -7.356 -7.355 0.001

BaHCO3+ 1.561e-008 1.412e-008 -7.807 -7.850 -0.044

BaCO3 2.286e-009 2.291e-009 -8.641 -8.640 0.001

BaOH+ 1.156e-012 1.046e-012 -11.937 -11.981 -0.044

C(4) 6.063e-003

HCO3- 5.697e-003 5.170e-003 -2.244 -2.286 -0.042

CO2 1.895e-004 1.899e-004 -3.722 -3.721 0.001

CaHCO3+ 8.663e-005 7.862e-005 -4.062 -4.104 -0.042

MgHCO3+ 3.445e-005 3.116e-005 -4.463 -4.506 -0.044

CaCO3 2.866e-005 2.872e-005 -4.543 -4.542 0.001

CO3-2 2.001e-005 1.358e-005 -4.699 -4.867 -0.169

MgCO3 5.750e-006 5.763e-006 -5.240 -5.239 0.001

NaHCO3 7.392e-007 7.409e-007 -6.131 -6.130 0.001

SrHCO3+ 3.358e-007 3.048e-007 -6.474 -6.516 -0.042

NaCO3- 3.790e-008 3.428e-008 -7.421 -7.465 -0.044

SrCO3 3.526e-008 3.534e-008 -7.453 -7.452 0.001

BaHCO3+ 1.561e-008 1.412e-008 -7.807 -7.850 -0.044

BaCO3 2.286e-009 2.291e-009 -8.641 -8.640 0.001

Ca 2.401e-003

Ca+2 2.229e-003 1.511e-003 -2.652 -2.821 -0.169

CaHCO3+ 8.663e-005 7.862e-005 -4.062 -4.104 -0.042

CaSO4 5.680e-005 5.693e-005 -4.246 -4.245 0.001

CaCO3 2.866e-005 2.872e-005 -4.543 -4.542 0.001

CaOH+ 2.058e-008 1.862e-008 -7.687 -7.730 -0.044

CaHSO4+ 4.354e-012 3.939e-012 -11.361 -11.405 -0.044

Cl 7.676e-005

Cl- 7.676e-005 6.932e-005 -4.115 -4.159 -0.044

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -44.238 -44.237 0.001

K 1.510e-005

K+ 1.508e-005 1.362e-005 -4.822 -4.866 -0.044

KSO4- 1.804e-008 1.632e-008 -7.744 -7.787 -0.044

KOH 3.496e-012 3.504e-012 -11.456 -11.455 0.001

Li 2.884e-006

Li+ 2.881e-006 2.619e-006 -5.540 -5.582 -0.041

LiSO4- 2.681e-009 2.425e-009 -8.572 -8.615 -0.044

LiOH 4.443e-012 4.453e-012 -11.352 -11.351 0.001

Mg 8.437e-004

Mg+2 7.842e-004 5.349e-004 -3.106 -3.272 -0.166

MgHCO3+ 3.445e-005 3.116e-005 -4.463 -4.506 -0.044

MgSO4 1.924e-005 1.928e-005 -4.716 -4.715 0.001

MgCO3 5.750e-006 5.763e-006 -5.240 -5.239 0.001

MgOH+ 5.153e-008 4.661e-008 -7.288 -7.332 -0.044

Na 2.824e-004

Na+ 2.814e-004 2.548e-004 -3.551 -3.594 -0.043

NaHCO3 7.392e-007 7.409e-007 -6.131 -6.130 0.001

NaSO4- 2.767e-007 2.503e-007 -6.558 -6.602 -0.044

NaCO3- 3.790e-008 3.428e-008 -7.421 -7.465 -0.044

NaOH 1.247e-010 1.250e-010 -9.904 -9.903 0.001

O(0) 2.287e-008

O2 1.143e-008 1.146e-008 -7.942 -7.941 0.001

S(6) 3.910e-004

SO4-2 3.144e-004 2.122e-004 -3.503 -3.673 -0.171

CaSO4 5.680e-005 5.693e-005 -4.246 -4.245 0.001

MgSO4 1.924e-005 1.928e-005 -4.716 -4.715 0.001

NaSO4- 2.767e-007 2.503e-007 -6.558 -6.602 -0.044

SrSO4 2.070e-007 2.075e-007 -6.684 -6.683 0.001

BaSO4 4.411e-008 4.420e-008 -7.356 -7.355 0.001

KSO4- 1.804e-008 1.632e-008 -7.744 -7.787 -0.044

LiSO4- 2.681e-009 2.425e-009 -8.572 -8.615 -0.044

HSO4- 2.396e-010 2.168e-010 -9.620 -9.664 -0.044

CaHSO4+ 4.354e-012 3.939e-012 -11.361 -11.405 -0.044

Si 7.327e-005

H4SiO4 7.271e-005 7.287e-005 -4.138 -4.137 0.001

H3SiO4- 5.612e-007 5.076e-007 -6.251 -6.294 -0.044

H2SiO4-2 1.654e-012 1.107e-012 -11.782 -11.956 -0.174

Sr 9.135e-006

Sr+2 8.557e-006 5.812e-006 -5.068 -5.236 -0.168

SrHCO3+ 3.358e-007 3.048e-007 -6.474 -6.516 -0.042

SrSO4 2.070e-007 2.075e-007 -6.684 -6.683 0.001

SrCO3 3.526e-008 3.534e-008 -7.453 -7.452 0.001

SrOH+ 2.440e-011 2.212e-011 -10.613 -10.655 -0.043

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.16 -6.49 -4.33 CaSO4

Aragonite 0.58 -7.69 -8.27 CaCO3

Barite 0.13 -10.05 -10.18 BaSO4

Calcite 0.73 -7.69 -8.42 CaCO3

Celestite -2.29 -8.91 -6.62 SrSO4

Chalcedony -0.44 -4.14 -3.70 SiO2

Chrysotile -4.61 29.13 33.75 Mg3Si2O5(OH)4

CO2(g) -2.41 -3.72 -1.31 CO2

Dolomite 0.97 -15.83 -16.80 CaMg(CO3)2

Gypsum -1.91 -6.49 -4.59 CaSO4:2H2O

H2(g) -41.14 -44.24 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.31 -7.75 1.55 NaCl

O2(g) -5.15 -7.94 -2.79 O2

Quartz 0.03 -4.14 -4.16 SiO2

Sepiolite -3.56 12.53 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -6.13 12.53 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.32 -4.14 -2.81 SiO2

Strontianite -0.82 -10.10 -9.28 SrCO3

Talc -1.96 20.86 22.82 Mg3Si4O10(OH)2

Witherite -2.64 -11.25 -8.61 BaCO3

Initial solution 11. 07-4-22

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 1.112e-007 1.112e-007

Alkalinity 5.755e-003 5.755e-003

B 2.684e-006 2.684e-006

Ba 6.556e-007 6.556e-007

Ca 2.222e-003 2.222e-003

Cl 8.325e-005 8.325e-005

K 1.817e-005 1.817e-005

Li 3.605e-006 3.605e-006

Mg 7.819e-004 7.819e-004

Na 1.941e-004 1.941e-004

S(6) 2.248e-004 2.248e-004

Si 8.492e-005 8.492e-005

Sr 1.039e-005 1.039e-005

----------------------------Description of solution----------------------------

pH = 7.789 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 415

Density (g/cm3) = 0.99979

Activity of water = 1.000

Ionic strength = 9.046e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 5.935e-003

Total CO2 (mol/kg) = 5.935e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -4.250e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.35

Iterations = 10

Total H = 1.110185e+002

Total O = 5.552505e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.580e-007 2.338e-007 -6.588 -6.631 -0.043

H+ 1.771e-008 1.626e-008 -7.752 -7.789 -0.037

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 1.112e-007

Al(OH)4- 1.100e-007 9.982e-008 -6.959 -7.001 -0.042

Al(OH)3 9.693e-010 9.713e-010 -9.014 -9.013 0.001

Al(OH)2+ 3.082e-010 2.797e-010 -9.511 -9.553 -0.042

AlOH+2 2.637e-012 1.790e-012 -11.579 -11.747 -0.168

Al+3 1.410e-014 6.531e-015 -13.851 -14.185 -0.334

AlSO4+ 2.410e-015 2.188e-015 -14.618 -14.660 -0.042

Al(SO4)2- 8.957e-018 8.131e-018 -17.048 -17.090 -0.042

AlHSO4+2 4.262e-024 2.894e-024 -23.370 -23.539 -0.168

B 2.684e-006

H3BO3 2.603e-006 2.609e-006 -5.585 -5.584 0.001

H2BO3- 8.094e-008 7.347e-008 -7.092 -7.134 -0.042

Ba 6.556e-007

Ba+2 6.123e-007 4.192e-007 -6.213 -6.378 -0.165

BaSO4 2.611e-008 2.617e-008 -7.583 -7.582 0.001

BaHCO3+ 1.535e-008 1.393e-008 -7.814 -7.856 -0.042

BaCO3 1.869e-009 1.872e-009 -8.728 -8.728 0.001

BaOH+ 9.621e-013 8.733e-013 -12.017 -12.059 -0.042

C(4) 5.935e-003

HCO3- 5.556e-003 5.059e-003 -2.255 -2.296 -0.041

CO2 2.239e-004 2.244e-004 -3.650 -3.649 0.001

CaHCO3+ 8.017e-005 7.300e-005 -4.096 -4.137 -0.041

MgHCO3+ 3.188e-005 2.894e-005 -4.496 -4.539 -0.042

CaCO3 2.204e-005 2.209e-005 -4.657 -4.656 0.001

CO3-2 1.601e-005 1.100e-005 -4.796 -4.959 -0.163

MgCO3 4.424e-006 4.433e-006 -5.354 -5.353 0.001

NaHCO3 4.990e-007 5.001e-007 -6.302 -6.301 0.001

SrHCO3+ 3.814e-007 3.473e-007 -6.419 -6.459 -0.041

SrCO3 3.328e-008 3.335e-008 -7.478 -7.477 0.001

NaCO3- 2.112e-008 1.917e-008 -7.675 -7.717 -0.042

BaHCO3+ 1.535e-008 1.393e-008 -7.814 -7.856 -0.042

BaCO3 1.869e-009 1.872e-009 -8.728 -8.728 0.001

Ca 2.222e-003

Ca+2 2.088e-003 1.434e-003 -2.680 -2.843 -0.163

CaHCO3+ 8.017e-005 7.300e-005 -4.096 -4.137 -0.041

CaSO4 3.165e-005 3.172e-005 -4.500 -4.499 0.001

CaCO3 2.204e-005 2.209e-005 -4.657 -4.656 0.001

CaOH+ 1.612e-008 1.464e-008 -7.793 -7.835 -0.042

CaHSO4+ 2.918e-012 2.649e-012 -11.535 -11.577 -0.042

Cl 8.325e-005

Cl- 8.325e-005 7.545e-005 -4.080 -4.122 -0.043

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -44.075 -44.074 0.001

K 1.817e-005

K+ 1.815e-005 1.645e-005 -4.741 -4.784 -0.043

KSO4- 1.275e-008 1.158e-008 -7.894 -7.936 -0.042

KOH 3.500e-012 3.508e-012 -11.456 -11.455 0.001

Li 3.605e-006

Li+ 3.603e-006 3.285e-006 -5.443 -5.483 -0.040

LiSO4- 1.968e-009 1.786e-009 -8.706 -8.748 -0.042

LiOH 4.618e-012 4.627e-012 -11.336 -11.335 0.001

Mg 7.819e-004

Mg+2 7.348e-004 5.077e-004 -3.134 -3.294 -0.161

MgHCO3+ 3.188e-005 2.894e-005 -4.496 -4.539 -0.042

MgSO4 1.072e-005 1.074e-005 -4.970 -4.969 0.001

MgCO3 4.424e-006 4.433e-006 -5.354 -5.353 0.001

MgOH+ 4.037e-008 3.665e-008 -7.394 -7.436 -0.042

Na 1.941e-004

Na+ 1.935e-004 1.758e-004 -3.713 -3.755 -0.042

NaHCO3 4.990e-007 5.001e-007 -6.302 -6.301 0.001

NaSO4- 1.117e-007 1.014e-007 -6.952 -6.994 -0.042

NaCO3- 2.112e-008 1.917e-008 -7.675 -7.717 -0.042

NaOH 7.126e-011 7.141e-011 -10.147 -10.146 0.001

O(0) 1.077e-008

O2 5.384e-009 5.395e-009 -8.269 -8.268 0.001

S(6) 2.248e-004

SO4-2 1.821e-004 1.246e-004 -3.740 -3.905 -0.165

CaSO4 3.165e-005 3.172e-005 -4.500 -4.499 0.001

MgSO4 1.072e-005 1.074e-005 -4.970 -4.969 0.001

SrSO4 1.416e-007 1.419e-007 -6.849 -6.848 0.001

NaSO4- 1.117e-007 1.014e-007 -6.952 -6.994 -0.042

BaSO4 2.611e-008 2.617e-008 -7.583 -7.582 0.001

KSO4- 1.275e-008 1.158e-008 -7.894 -7.936 -0.042

LiSO4- 1.968e-009 1.786e-009 -8.706 -8.748 -0.042

HSO4- 1.692e-010 1.536e-010 -9.772 -9.814 -0.042

CaHSO4+ 2.918e-012 2.649e-012 -11.535 -11.577 -0.042

AlSO4+ 2.410e-015 2.188e-015 -14.618 -14.660 -0.042

Al(SO4)2- 8.957e-018 8.131e-018 -17.048 -17.090 -0.042

AlHSO4+2 4.262e-024 2.894e-024 -23.370 -23.539 -0.168

Si 8.492e-005

H4SiO4 8.439e-005 8.456e-005 -4.074 -4.073 0.001

H3SiO4- 5.375e-007 4.879e-007 -6.270 -6.312 -0.042

H2SiO4-2 1.298e-012 8.815e-013 -11.887 -12.055 -0.168

Sr 1.039e-005

Sr+2 9.835e-006 6.768e-006 -5.007 -5.170 -0.162

SrHCO3+ 3.814e-007 3.473e-007 -6.419 -6.459 -0.041

SrSO4 1.416e-007 1.419e-007 -6.849 -6.848 0.001

SrCO3 3.328e-008 3.335e-008 -7.478 -7.477 0.001

SrOH+ 2.346e-011 2.134e-011 -10.630 -10.671 -0.041

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -2.43 9.18 11.61 Al(OH)3

Albite -4.18 -22.97 -18.80 NaAlSi3O8

Alunite -8.56 -8.42 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.41 -6.75 -4.33 CaSO4

Anorthite -4.92 -24.99 -20.07 CaAl2Si2O8

Aragonite 0.47 -7.80 -8.27 CaCO3

Barite -0.10 -10.28 -10.18 BaSO4

Ca-Montmorillonite -0.48 -47.31 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.62 -7.80 -8.42 CaCO3

Celestite -2.45 -9.07 -6.62 SrSO4

Chalcedony -0.38 -4.07 -3.70 SiO2

Chlorite(14A) -5.48 67.56 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -5.04 28.70 33.75 Mg3Si2O5(OH)4

CO2(g) -2.34 -3.65 -1.31 CO2

Dolomite 0.75 -16.05 -16.80 CaMg(CO3)2

Gibbsite 0.37 9.18 8.81 Al(OH)3

Gypsum -2.16 -6.75 -4.59 CaSO4:2H2O

H2(g) -40.98 -44.07 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.43 -7.88 1.55 NaCl

Illite -1.45 -43.40 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -2.48 -24.00 -21.52 KAlSi3O8

K-mica 3.80 18.33 14.53 KAl3Si3O10(OH)2

Kaolinite 1.70 10.22 8.52 Al2Si2O5(OH)4

O2(g) -5.47 -8.27 -2.79 O2

Quartz 0.09 -4.07 -4.16 SiO2

Sepiolite -3.74 12.35 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -6.31 12.35 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.26 -4.07 -2.81 SiO2

Strontianite -0.85 -10.13 -9.28 SrCO3

Talc -2.26 20.56 22.82 Mg3Si4O10(OH)2

Witherite -2.73 -11.34 -8.61 BaCO3

Initial solution 12. 07-6-4

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 5.788e-003 5.788e-003

B 3.147e-006 3.147e-006

Ba 6.483e-007 6.483e-007

Ca 2.187e-003 2.187e-003

Cl 7.309e-005 7.309e-005

K 2.124e-005 2.124e-005

Li 3.749e-006 3.749e-006

Mg 8.354e-004 8.354e-004

N(5) 1.357e-006 1.357e-006

Na 2.076e-004 2.076e-004

S(6) 2.123e-004 2.123e-004

Si 9.658e-005 9.658e-005

Sr 1.176e-005 1.176e-005

----------------------------Description of solution----------------------------

pH = 7.541 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 417

Density (g/cm3) = 0.99979

Activity of water = 1.000

Ionic strength = 9.112e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.164e-003

Total CO2 (mol/kg) = 6.164e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = 1.470e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.12

Iterations = 9

Total H = 1.110186e+002

Total O = 5.552556e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.459e-007 1.322e-007 -6.836 -6.879 -0.043

H+ 3.134e-008 2.877e-008 -7.504 -7.541 -0.037

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 3.147e-006

H3BO3 3.092e-006 3.099e-006 -5.510 -5.509 0.001

H2BO3- 5.437e-008 4.934e-008 -7.265 -7.307 -0.042

Ba 6.483e-007

Ba+2 6.075e-007 4.154e-007 -6.216 -6.382 -0.165

BaSO4 2.437e-008 2.442e-008 -7.613 -7.612 0.001

BaHCO3+ 1.540e-008 1.397e-008 -7.813 -7.855 -0.042

BaCO3 1.059e-009 1.061e-009 -8.975 -8.974 0.001

BaOH+ 5.391e-013 4.892e-013 -12.268 -12.310 -0.042

C(4) 6.164e-003

HCO3- 5.623e-003 5.118e-003 -2.250 -2.291 -0.041

CO2 4.007e-004 4.016e-004 -3.397 -3.396 0.001

CaHCO3+ 8.015e-005 7.296e-005 -4.096 -4.137 -0.041

MgHCO3+ 3.453e-005 3.134e-005 -4.462 -4.504 -0.042

CaCO3 1.245e-005 1.248e-005 -4.905 -4.904 0.001

CO3-2 9.165e-006 6.293e-006 -5.038 -5.201 -0.163

MgCO3 2.708e-006 2.714e-006 -5.567 -5.566 0.001

NaHCO3 5.399e-007 5.410e-007 -6.268 -6.267 0.001

SrHCO3+ 4.372e-007 3.980e-007 -6.359 -6.400 -0.041

SrCO3 2.156e-008 2.160e-008 -7.666 -7.665 0.001

BaHCO3+ 1.540e-008 1.397e-008 -7.813 -7.855 -0.042

NaCO3- 1.292e-008 1.172e-008 -7.889 -7.931 -0.042

BaCO3 1.059e-009 1.061e-009 -8.975 -8.974 0.001

Ca 2.187e-003

Ca+2 2.065e-003 1.417e-003 -2.685 -2.849 -0.164

CaHCO3+ 8.015e-005 7.296e-005 -4.096 -4.137 -0.041

CaSO4 2.944e-005 2.951e-005 -4.531 -4.530 0.001

CaCO3 1.245e-005 1.248e-005 -4.905 -4.904 0.001

CaOH+ 9.005e-009 8.171e-009 -8.046 -8.088 -0.042

CaHSO4+ 4.804e-012 4.360e-012 -11.318 -11.361 -0.042

Cl 7.309e-005

Cl- 7.309e-005 6.622e-005 -4.136 -4.179 -0.043

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.579 -43.578 0.001

K 2.124e-005

K+ 2.122e-005 1.923e-005 -4.673 -4.716 -0.043

KSO4- 1.404e-008 1.274e-008 -7.853 -7.895 -0.042

KOH 2.312e-012 2.317e-012 -11.636 -11.635 0.001

Li 3.749e-006

Li+ 3.747e-006 3.416e-006 -5.426 -5.467 -0.040

LiSO4- 1.928e-009 1.749e-009 -8.715 -8.757 -0.042

LiOH 2.714e-012 2.720e-012 -11.566 -11.566 0.001

Mg 8.354e-004

Mg+2 7.873e-004 5.434e-004 -3.104 -3.265 -0.161

MgHCO3+ 3.453e-005 3.134e-005 -4.462 -4.504 -0.042

MgSO4 1.081e-005 1.083e-005 -4.966 -4.965 0.001

MgCO3 2.708e-006 2.714e-006 -5.567 -5.566 0.001

MgOH+ 2.443e-008 2.217e-008 -7.612 -7.654 -0.042

N(5) 1.357e-006

NO3- 1.357e-006 1.227e-006 -5.867 -5.911 -0.044

Na 2.076e-004

Na+ 2.069e-004 1.880e-004 -3.684 -3.726 -0.042

NaHCO3 5.399e-007 5.410e-007 -6.268 -6.267 0.001

NaSO4- 1.125e-007 1.021e-007 -6.949 -6.991 -0.042

NaCO3- 1.292e-008 1.172e-008 -7.889 -7.931 -0.042

NaOH 4.307e-011 4.316e-011 -10.366 -10.365 0.001

O(0) 1.099e-009

O2 5.496e-010 5.508e-010 -9.260 -9.259 0.001

S(6) 2.123e-004

SO4-2 1.717e-004 1.173e-004 -3.765 -3.931 -0.165

CaSO4 2.944e-005 2.951e-005 -4.531 -4.530 0.001

MgSO4 1.081e-005 1.083e-005 -4.966 -4.965 0.001

SrSO4 1.510e-007 1.513e-007 -6.821 -6.820 0.001

NaSO4- 1.125e-007 1.021e-007 -6.949 -6.991 -0.042

BaSO4 2.437e-008 2.442e-008 -7.613 -7.612 0.001

KSO4- 1.404e-008 1.274e-008 -7.853 -7.895 -0.042

LiSO4- 1.928e-009 1.749e-009 -8.715 -8.757 -0.042

HSO4- 2.821e-010 2.560e-010 -9.550 -9.592 -0.042

CaHSO4+ 4.804e-012 4.360e-012 -11.318 -11.361 -0.042

Si 9.658e-005

H4SiO4 9.623e-005 9.643e-005 -4.017 -4.016 0.001

H3SiO4- 3.466e-007 3.145e-007 -6.460 -6.502 -0.042

H2SiO4-2 4.737e-013 3.212e-013 -12.325 -12.493 -0.169

Sr 1.176e-005

Sr+2 1.115e-005 7.665e-006 -4.953 -5.115 -0.163

SrHCO3+ 4.372e-007 3.980e-007 -6.359 -6.400 -0.041

SrSO4 1.510e-007 1.513e-007 -6.821 -6.820 0.001

SrCO3 2.156e-008 2.160e-008 -7.666 -7.665 0.001

SrOH+ 1.502e-011 1.366e-011 -10.823 -10.864 -0.041

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.45 -6.78 -4.33 CaSO4

Aragonite 0.22 -8.05 -8.27 CaCO3

Barite -0.13 -10.31 -10.18 BaSO4

Calcite 0.37 -8.05 -8.42 CaCO3

Celestite -2.42 -9.05 -6.62 SrSO4

Chalcedony -0.32 -4.02 -3.70 SiO2

Chrysotile -6.33 27.42 33.75 Mg3Si2O5(OH)4

CO2(g) -2.08 -3.40 -1.31 CO2

Dolomite 0.28 -16.52 -16.80 CaMg(CO3)2

Gypsum -2.19 -6.78 -4.59 CaSO4:2H2O

H2(g) -40.48 -43.58 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.46 -7.90 1.55 NaCl

O2(g) -6.46 -9.26 -2.79 O2

Quartz 0.15 -4.02 -4.16 SiO2

Sepiolite -4.50 11.59 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -7.07 11.59 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.20 -4.02 -2.81 SiO2

Strontianite -1.04 -10.32 -9.28 SrCO3

Talc -3.43 19.39 22.82 Mg3Si4O10(OH)2

Witherite -2.97 -11.58 -8.61 BaCO3

Initial solution 13. 07-7-24

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 6.100e-003 6.100e-003

B 3.795e-006 3.795e-006

Ba 6.484e-007 6.484e-007

Ca 2.344e-003 2.344e-003

Cl 8.579e-005 8.579e-005

K 2.508e-005 2.508e-005

Li 4.326e-006 4.326e-006

Mg 8.972e-004 8.972e-004

N(5) 2.786e-006 2.786e-006

Na 2.254e-004 2.254e-004

S(6) 3.170e-004 3.170e-004

Si 1.032e-004 1.032e-004

Sr 1.347e-005 1.347e-005

----------------------------Description of solution----------------------------

pH = 7.229 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 450

Density (g/cm3) = 0.99982

Activity of water = 1.000

Ionic strength = 9.839e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.954e-003

Total CO2 (mol/kg) = 6.954e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -5.684e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.44

Iterations = 9

Total H = 1.110189e+002

Total O = 5.552791e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 7.131e-008 6.436e-008 -7.147 -7.191 -0.045

H+ 6.453e-008 5.907e-008 -7.190 -7.229 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 3.795e-006

H3BO3 3.762e-006 3.771e-006 -5.425 -5.424 0.001

H2BO3- 3.233e-008 2.924e-008 -7.490 -7.534 -0.044

Ba 6.484e-007

Ba+2 5.974e-007 4.033e-007 -6.224 -6.394 -0.171

BaSO4 3.462e-008 3.470e-008 -7.461 -7.460 0.001

BaHCO3+ 1.580e-008 1.429e-008 -7.801 -7.845 -0.044

BaCO3 5.277e-010 5.289e-010 -9.278 -9.277 0.001

BaOH+ 2.558e-013 2.313e-013 -12.592 -12.636 -0.044

C(4) 6.954e-003

HCO3- 5.945e-003 5.394e-003 -2.226 -2.268 -0.042

CO2 8.671e-004 8.690e-004 -3.062 -3.061 0.001

CaHCO3+ 8.927e-005 8.101e-005 -4.049 -4.091 -0.042

MgHCO3+ 3.851e-005 3.483e-005 -4.414 -4.458 -0.044

CaCO3 6.733e-006 6.748e-006 -5.172 -5.171 0.001

CO3-2 4.764e-006 3.230e-006 -5.322 -5.491 -0.169

MgCO3 1.466e-006 1.469e-006 -5.834 -5.833 0.001

NaHCO3 6.156e-007 6.170e-007 -6.211 -6.210 0.001

SrHCO3+ 5.196e-007 4.715e-007 -6.284 -6.326 -0.042

BaHCO3+ 1.580e-008 1.429e-008 -7.801 -7.845 -0.044

SrCO3 1.244e-008 1.247e-008 -7.905 -7.904 0.001

NaCO3- 7.199e-009 6.511e-009 -8.143 -8.186 -0.044

BaCO3 5.277e-010 5.289e-010 -9.278 -9.277 0.001

Ca 2.344e-003

Ca+2 2.203e-003 1.493e-003 -2.657 -2.826 -0.169

CaHCO3+ 8.927e-005 8.101e-005 -4.049 -4.091 -0.042

CaSO4 4.538e-005 4.549e-005 -4.343 -4.342 0.001

CaCO3 6.733e-006 6.748e-006 -5.172 -5.171 0.001

CaOH+ 4.636e-009 4.193e-009 -8.334 -8.378 -0.044

CaHSO4+ 1.526e-011 1.380e-011 -10.816 -10.860 -0.044

Cl 8.579e-005

Cl- 8.579e-005 7.746e-005 -4.067 -4.111 -0.044

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -42.954 -42.953 0.001

K 2.508e-005

K+ 2.505e-005 2.262e-005 -4.601 -4.646 -0.044

KSO4- 2.425e-008 2.193e-008 -7.615 -7.659 -0.044

KOH 1.324e-012 1.327e-012 -11.878 -11.877 0.001

Li 4.326e-006

Li+ 4.322e-006 3.929e-006 -5.364 -5.406 -0.042

LiSO4- 3.255e-009 2.944e-009 -8.488 -8.531 -0.044

LiOH 1.520e-012 1.523e-012 -11.818 -11.817 0.001

Mg 8.972e-004

Mg+2 8.405e-004 5.731e-004 -3.075 -3.242 -0.166

MgHCO3+ 3.851e-005 3.483e-005 -4.414 -4.458 -0.044

MgSO4 1.667e-005 1.671e-005 -4.778 -4.777 0.001

MgCO3 1.466e-006 1.469e-006 -5.834 -5.833 0.001

MgOH+ 1.259e-008 1.139e-008 -7.900 -7.944 -0.044

N(5) 2.786e-006

NO3- 2.786e-006 2.511e-006 -5.555 -5.600 -0.045

Na 2.254e-004

Na+ 2.246e-004 2.034e-004 -3.649 -3.692 -0.043

NaHCO3 6.156e-007 6.170e-007 -6.211 -6.210 0.001

NaSO4- 1.787e-007 1.616e-007 -6.748 -6.791 -0.044

NaCO3- 7.199e-009 6.511e-009 -8.143 -8.186 -0.044

NaOH 2.269e-011 2.275e-011 -10.644 -10.643 0.001

O(0) 6.183e-011

O2 3.091e-011 3.098e-011 -10.510 -10.509 0.001

S(6) 3.170e-004

SO4-2 2.545e-004 1.717e-004 -3.594 -3.765 -0.171

CaSO4 4.538e-005 4.549e-005 -4.343 -4.342 0.001

MgSO4 1.667e-005 1.671e-005 -4.778 -4.777 0.001

SrSO4 2.484e-007 2.489e-007 -6.605 -6.604 0.001

NaSO4- 1.787e-007 1.616e-007 -6.748 -6.791 -0.044

BaSO4 3.462e-008 3.470e-008 -7.461 -7.460 0.001

KSO4- 2.425e-008 2.193e-008 -7.615 -7.659 -0.044

LiSO4- 3.255e-009 2.944e-009 -8.488 -8.531 -0.044

HSO4- 8.503e-010 7.690e-010 -9.070 -9.114 -0.044

CaHSO4+ 1.526e-011 1.380e-011 -10.816 -10.860 -0.044

Si 1.032e-004

H4SiO4 1.031e-004 1.033e-004 -3.987 -3.986 0.001

H3SiO4- 1.814e-007 1.641e-007 -6.741 -6.785 -0.044

H2SiO4-2 1.219e-013 8.160e-014 -12.914 -13.088 -0.174

Sr 1.347e-005

Sr+2 1.269e-005 8.618e-006 -4.896 -5.065 -0.168

SrHCO3+ 5.196e-007 4.715e-007 -6.284 -6.326 -0.042

SrSO4 2.484e-007 2.489e-007 -6.605 -6.604 0.001

SrCO3 1.244e-008 1.247e-008 -7.905 -7.904 0.001

SrOH+ 8.253e-012 7.481e-012 -11.083 -11.126 -0.043

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.26 -6.59 -4.33 CaSO4

Aragonite -0.05 -8.32 -8.27 CaCO3

Barite 0.02 -10.16 -10.18 BaSO4

Calcite 0.11 -8.32 -8.42 CaCO3

Celestite -2.21 -8.83 -6.62 SrSO4

Chalcedony -0.29 -3.99 -3.70 SiO2

Chrysotile -8.07 25.67 33.75 Mg3Si2O5(OH)4

CO2(g) -1.75 -3.06 -1.31 CO2

Dolomite -0.25 -17.05 -16.80 CaMg(CO3)2

Gypsum -2.00 -6.59 -4.59 CaSO4:2H2O

H2(g) -39.86 -42.95 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.36 -7.80 1.55 NaCl

O2(g) -7.71 -10.51 -2.79 O2

Quartz 0.18 -3.99 -4.16 SiO2

Sepiolite -5.62 10.47 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.19 10.47 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.17 -3.99 -2.81 SiO2

Strontianite -1.28 -10.56 -9.28 SrCO3

Talc -5.12 17.70 22.82 Mg3Si4O10(OH)2

Witherite -3.27 -11.89 -8.61 BaCO3

Initial solution 14. 07-8-26

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 4.821e-007 4.821e-007

Alkalinity 6.034e-003 6.034e-003

B 3.980e-006 3.980e-006

Ba 6.047e-007 6.047e-007

Ca 2.374e-003 2.374e-003

Cl 7.958e-005 7.958e-005

K 2.687e-005 2.687e-005

Li 4.614e-006 4.614e-006

Mg 9.260e-004 9.260e-004

N(5) 1.714e-006 1.714e-006

Na 2.337e-004 2.337e-004

S(6) 3.636e-004 3.636e-004

Si 1.099e-004 1.099e-004

Sr 1.427e-005 1.427e-005

----------------------------Description of solution----------------------------

pH = 7.126 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 455

Density (g/cm3) = 0.99983

Activity of water = 1.000

Ionic strength = 9.983e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.109e-003

Total CO2 (mol/kg) = 7.109e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = 5.375e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.41

Iterations = 11

Total H = 1.110189e+002

Total O = 5.552837e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

H+ 8.183e-008 7.487e-008 -7.087 -7.126 -0.039

OH- 5.630e-008 5.078e-008 -7.250 -7.294 -0.045

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 4.821e-007

Al(OH)4- 4.373e-007 3.953e-007 -6.359 -6.403 -0.044

Al(OH)2+ 2.598e-008 2.349e-008 -7.585 -7.629 -0.044

Al(OH)3 1.767e-008 1.771e-008 -7.753 -7.752 0.001

AlOH+2 1.037e-009 6.921e-010 -8.984 -9.160 -0.176

Al+3 2.587e-011 1.163e-011 -10.587 -10.935 -0.347

AlSO4+ 6.777e-012 6.125e-012 -11.169 -11.213 -0.044

Al(SO4)2- 3.962e-014 3.581e-014 -13.402 -13.446 -0.044

AlHSO4+2 5.589e-020 3.731e-020 -19.253 -19.428 -0.176

B 3.980e-006

H3BO3 3.953e-006 3.962e-006 -5.403 -5.402 0.001

H2BO3- 2.682e-008 2.424e-008 -7.572 -7.615 -0.044

Ba 6.047e-007

Ba+2 5.533e-007 3.726e-007 -6.257 -6.429 -0.172

BaSO4 3.651e-008 3.659e-008 -7.438 -7.437 0.001

BaHCO3+ 1.445e-008 1.306e-008 -7.840 -7.884 -0.044

BaCO3 3.803e-010 3.812e-010 -9.420 -9.419 0.001

BaOH+ 1.865e-013 1.686e-013 -12.729 -12.773 -0.044

C(4) 7.109e-003

HCO3- 5.882e-003 5.334e-003 -2.230 -2.273 -0.042

CO2 1.087e-003 1.089e-003 -2.964 -2.963 0.001

CaHCO3+ 8.911e-005 8.081e-005 -4.050 -4.093 -0.042

MgHCO3+ 3.918e-005 3.541e-005 -4.407 -4.451 -0.044

CaCO3 5.299e-006 5.311e-006 -5.276 -5.275 0.001

CO3-2 3.725e-006 2.520e-006 -5.429 -5.599 -0.170

MgCO3 1.175e-006 1.178e-006 -5.930 -5.929 0.001

NaHCO3 6.306e-007 6.321e-007 -6.200 -6.199 0.001

SrHCO3+ 5.424e-007 4.919e-007 -6.266 -6.308 -0.042

BaHCO3+ 1.445e-008 1.306e-008 -7.840 -7.884 -0.044

SrCO3 1.024e-008 1.026e-008 -7.990 -7.989 0.001

NaCO3- 5.822e-009 5.262e-009 -8.235 -8.279 -0.044

BaCO3 3.803e-010 3.812e-010 -9.420 -9.419 0.001

Ca 2.374e-003

Ca+2 2.227e-003 1.506e-003 -2.652 -2.822 -0.170

CaHCO3+ 8.911e-005 8.081e-005 -4.050 -4.093 -0.042

CaSO4 5.225e-005 5.237e-005 -4.282 -4.281 0.001

CaCO3 5.299e-006 5.311e-006 -5.276 -5.275 0.001

CaOH+ 3.692e-009 3.337e-009 -8.433 -8.477 -0.044

CaHSO4+ 2.228e-011 2.014e-011 -10.652 -10.696 -0.044

Cl 7.958e-005

Cl- 7.958e-005 7.181e-005 -4.099 -4.144 -0.045

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -42.748 -42.747 0.001

K 2.687e-005

K+ 2.684e-005 2.421e-005 -4.571 -4.616 -0.045

KSO4- 2.965e-008 2.680e-008 -7.528 -7.572 -0.044

KOH 1.119e-012 1.121e-012 -11.951 -11.950 0.001

Li 4.614e-006

Li+ 4.610e-006 4.188e-006 -5.336 -5.378 -0.042

LiSO4- 3.962e-009 3.581e-009 -8.402 -8.446 -0.044

LiOH 1.278e-012 1.281e-012 -11.893 -11.892 0.001

Mg 9.260e-004

Mg+2 8.660e-004 5.891e-004 -3.062 -3.230 -0.167

MgHCO3+ 3.918e-005 3.541e-005 -4.407 -4.451 -0.044

MgSO4 1.956e-005 1.961e-005 -4.709 -4.708 0.001

MgCO3 1.175e-006 1.178e-006 -5.930 -5.929 0.001

MgOH+ 1.022e-008 9.236e-009 -7.991 -8.035 -0.044

N(5) 1.714e-006

NO3- 1.714e-006 1.544e-006 -5.766 -5.811 -0.045

Na 2.337e-004

Na+ 2.329e-004 2.107e-004 -3.633 -3.676 -0.043

NaHCO3 6.306e-007 6.321e-007 -6.200 -6.199 0.001

NaSO4- 2.115e-007 1.911e-007 -6.675 -6.719 -0.044

NaCO3- 5.822e-009 5.262e-009 -8.235 -8.279 -0.044

NaOH 1.855e-011 1.859e-011 -10.732 -10.731 0.001

O(0) 2.395e-011

O2 1.198e-011 1.200e-011 -10.922 -10.921 0.001

S(6) 3.636e-004

SO4-2 2.912e-004 1.959e-004 -3.536 -3.708 -0.172

CaSO4 5.225e-005 5.237e-005 -4.282 -4.281 0.001

MgSO4 1.956e-005 1.961e-005 -4.709 -4.708 0.001

SrSO4 2.990e-007 2.997e-007 -6.524 -6.523 0.001

NaSO4- 2.115e-007 1.911e-007 -6.675 -6.719 -0.044

BaSO4 3.651e-008 3.659e-008 -7.438 -7.437 0.001

KSO4- 2.965e-008 2.680e-008 -7.528 -7.572 -0.044

LiSO4- 3.962e-009 3.581e-009 -8.402 -8.446 -0.044

HSO4- 1.231e-009 1.113e-009 -8.910 -8.954 -0.044

CaHSO4+ 2.228e-011 2.014e-011 -10.652 -10.696 -0.044

AlSO4+ 6.777e-012 6.125e-012 -11.169 -11.213 -0.044

Al(SO4)2- 3.962e-014 3.581e-014 -13.402 -13.446 -0.044

AlHSO4+2 5.589e-020 3.731e-020 -19.253 -19.428 -0.176

Si 1.099e-004

H4SiO4 1.098e-004 1.100e-004 -3.960 -3.959 0.001

H3SiO4- 1.525e-007 1.379e-007 -6.817 -6.861 -0.044

H2SiO4-2 8.104e-014 5.409e-014 -13.091 -13.267 -0.176

Sr 1.427e-005

Sr+2 1.342e-005 9.090e-006 -4.872 -5.041 -0.169

SrHCO3+ 5.424e-007 4.919e-007 -6.266 -6.308 -0.042

SrSO4 2.990e-007 2.997e-007 -6.524 -6.523 0.001

SrCO3 1.024e-008 1.026e-008 -7.990 -7.989 0.001

SrOH+ 6.872e-012 6.225e-012 -11.163 -11.206 -0.043

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -1.17 10.44 11.61 Al(OH)3

Albite -3.16 -21.95 -18.80 NaAlSi3O8

Alunite -2.23 -2.08 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.20 -6.53 -4.33 CaSO4

Anorthite -3.47 -23.54 -20.07 CaAl2Si2O8

Aragonite -0.15 -8.42 -8.27 CaCO3

Barite 0.05 -10.14 -10.18 BaSO4

Ca-Montmorillonite 2.66 -44.16 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.00 -8.42 -8.42 CaCO3

Celestite -2.13 -8.75 -6.62 SrSO4

Chalcedony -0.26 -3.96 -3.70 SiO2

Chlorite(14A) -8.92 64.12 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -8.60 25.15 33.75 Mg3Si2O5(OH)4

CO2(g) -1.65 -2.96 -1.31 CO2

Dolomite -0.45 -17.25 -16.80 CaMg(CO3)2

Gibbsite 1.63 10.44 8.81 Al(OH)3

Gypsum -1.94 -6.53 -4.59 CaSO4:2H2O

H2(g) -39.65 -42.75 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.37 -7.82 1.55 NaCl

Illite 1.24 -40.71 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -1.37 -22.89 -21.52 KAlSi3O8

K-mica 7.43 21.96 14.53 KAl3Si3O10(OH)2

Kaolinite 4.45 12.97 8.52 Al2Si2O5(OH)4

O2(g) -8.13 -10.92 -2.79 O2

Quartz 0.21 -3.96 -4.16 SiO2

Sepiolite -5.92 10.17 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.49 10.17 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.14 -3.96 -2.81 SiO2

Strontianite -1.36 -10.64 -9.28 SrCO3

Talc -5.59 17.23 22.82 Mg3Si4O10(OH)2

Witherite -3.42 -12.03 -8.61 BaCO3

Initial solution 15. 07-9-22

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 1.483e-006 1.483e-006

Alkalinity 6.133e-003 6.133e-003

B 5.276e-006 5.276e-006

Ba 6.848e-007 6.848e-007

Ca 2.407e-003 2.407e-003

Cl 7.648e-005 7.648e-005

K 2.661e-005 2.661e-005

Li 4.470e-006 4.470e-006

Mg 9.013e-004 9.013e-004

N(5) 3.786e-006 3.786e-006

Na 2.224e-004 2.224e-004

S(6) 3.761e-004 3.761e-004

Si 1.016e-004 1.016e-004

Sr 1.222e-005 1.222e-005

----------------------------Description of solution----------------------------

pH = 7.086 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 458

Density (g/cm3) = 0.99983

Activity of water = 1.000

Ionic strength = 1.005e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.327e-003

Total CO2 (mol/kg) = 7.327e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -6.574e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.50

Iterations = 11

Total H = 1.110190e+002

Total O = 5.552893e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

H+ 8.969e-008 8.204e-008 -7.047 -7.086 -0.039

OH- 5.139e-008 4.634e-008 -7.289 -7.334 -0.045

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 1.483e-006

Al(OH)4- 1.326e-006 1.198e-006 -5.878 -5.922 -0.044

Al(OH)2+ 9.458e-008 8.546e-008 -7.024 -7.068 -0.044

Al(OH)3 5.868e-008 5.881e-008 -7.232 -7.231 0.001

AlOH+2 4.140e-009 2.760e-009 -8.383 -8.559 -0.176

Al+3 1.133e-010 5.080e-011 -9.946 -10.294 -0.348

AlSO4+ 3.061e-011 2.766e-011 -10.514 -10.558 -0.044

Al(SO4)2- 1.850e-013 1.671e-013 -12.733 -12.777 -0.044

AlHSO4+2 2.769e-019 1.846e-019 -18.558 -18.734 -0.176

B 5.276e-006

H3BO3 5.243e-006 5.255e-006 -5.280 -5.279 0.001

H2BO3- 3.247e-008 2.934e-008 -7.489 -7.533 -0.044

Ba 6.848e-007

Ba+2 6.253e-007 4.206e-007 -6.204 -6.376 -0.172

BaSO4 4.259e-008 4.268e-008 -7.371 -7.370 0.001

BaHCO3+ 1.657e-008 1.497e-008 -7.781 -7.825 -0.044

BaCO3 3.979e-010 3.989e-010 -9.400 -9.399 0.001

BaOH+ 1.922e-013 1.737e-013 -12.716 -12.760 -0.044

C(4) 7.327e-003

HCO3- 5.976e-003 5.418e-003 -2.224 -2.266 -0.043

CO2 1.210e-003 1.212e-003 -2.917 -2.916 0.001

CaHCO3+ 9.157e-005 8.302e-005 -4.038 -4.081 -0.043

MgHCO3+ 3.866e-005 3.493e-005 -4.413 -4.457 -0.044

CaCO3 4.968e-006 4.980e-006 -5.304 -5.303 0.001

CO3-2 3.457e-006 2.336e-006 -5.461 -5.632 -0.170

MgCO3 1.058e-006 1.061e-006 -5.975 -5.974 0.001

NaHCO3 6.093e-007 6.107e-007 -6.215 -6.214 0.001

SrHCO3+ 4.706e-007 4.267e-007 -6.327 -6.370 -0.043

BaHCO3+ 1.657e-008 1.497e-008 -7.781 -7.825 -0.044

SrCO3 8.103e-009 8.122e-009 -8.091 -8.090 0.001

NaCO3- 5.135e-009 4.640e-009 -8.289 -8.333 -0.044

BaCO3 3.979e-010 3.989e-010 -9.400 -9.399 0.001

Ca 2.407e-003

Ca+2 2.255e-003 1.523e-003 -2.647 -2.817 -0.171

CaHCO3+ 9.157e-005 8.302e-005 -4.038 -4.081 -0.043

CaSO4 5.462e-005 5.475e-005 -4.263 -4.262 0.001

CaCO3 4.968e-006 4.980e-006 -5.304 -5.303 0.001

CaOH+ 3.409e-009 3.080e-009 -8.467 -8.511 -0.044

CaHSO4+ 2.553e-011 2.307e-011 -10.593 -10.637 -0.044

Cl 7.648e-005

Cl- 7.648e-005 6.899e-005 -4.116 -4.161 -0.045

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -42.669 -42.668 0.001

K 2.661e-005

K+ 2.658e-005 2.398e-005 -4.575 -4.620 -0.045

KSO4- 3.035e-008 2.743e-008 -7.518 -7.562 -0.044

KOH 1.011e-012 1.013e-012 -11.995 -11.994 0.001

Li 4.470e-006

Li+ 4.466e-006 4.056e-006 -5.350 -5.392 -0.042

LiSO4- 3.967e-009 3.585e-009 -8.402 -8.446 -0.044

LiOH 1.130e-012 1.132e-012 -11.947 -11.946 0.001

Mg 9.013e-004

Mg+2 8.419e-004 5.721e-004 -3.075 -3.243 -0.168

MgHCO3+ 3.866e-005 3.493e-005 -4.413 -4.457 -0.044

MgSO4 1.963e-005 1.968e-005 -4.707 -4.706 0.001

MgCO3 1.058e-006 1.061e-006 -5.975 -5.974 0.001

MgOH+ 9.058e-009 8.185e-009 -8.043 -8.087 -0.044

N(5) 3.786e-006

NO3- 3.786e-006 3.409e-006 -5.422 -5.467 -0.046

Na 2.224e-004

Na+ 2.216e-004 2.004e-004 -3.654 -3.698 -0.044

NaHCO3 6.093e-007 6.107e-007 -6.215 -6.214 0.001

NaSO4- 2.080e-007 1.879e-007 -6.682 -6.726 -0.044

NaCO3- 5.135e-009 4.640e-009 -8.289 -8.333 -0.044

NaOH 1.610e-011 1.614e-011 -10.793 -10.792 0.001

O(0) 1.661e-011

O2 8.306e-012 8.325e-012 -11.081 -11.080 0.001

S(6) 3.761e-004

SO4-2 3.013e-004 2.025e-004 -3.521 -3.694 -0.173

CaSO4 5.462e-005 5.475e-005 -4.263 -4.262 0.001

MgSO4 1.963e-005 1.968e-005 -4.707 -4.706 0.001

SrSO4 2.639e-007 2.646e-007 -6.578 -6.577 0.001

NaSO4- 2.080e-007 1.879e-007 -6.682 -6.726 -0.044

BaSO4 4.259e-008 4.268e-008 -7.371 -7.370 0.001

KSO4- 3.035e-008 2.743e-008 -7.518 -7.562 -0.044

LiSO4- 3.967e-009 3.585e-009 -8.402 -8.446 -0.044

HSO4- 1.394e-009 1.260e-009 -8.856 -8.900 -0.044

AlSO4+ 3.061e-011 2.766e-011 -10.514 -10.558 -0.044

CaHSO4+ 2.553e-011 2.307e-011 -10.593 -10.637 -0.044

Al(SO4)2- 1.850e-013 1.671e-013 -12.733 -12.777 -0.044

AlHSO4+2 2.769e-019 1.846e-019 -18.558 -18.734 -0.176

Si 1.016e-004

H4SiO4 1.015e-004 1.017e-004 -3.994 -3.993 0.001

H3SiO4- 1.287e-007 1.163e-007 -6.890 -6.934 -0.044

H2SiO4-2 6.246e-014 4.164e-014 -13.204 -13.380 -0.176

Sr 1.222e-005

Sr+2 1.148e-005 7.764e-006 -4.940 -5.110 -0.170

SrHCO3+ 4.706e-007 4.267e-007 -6.327 -6.370 -0.043

SrSO4 2.639e-007 2.646e-007 -6.578 -6.577 0.001

SrCO3 8.103e-009 8.122e-009 -8.091 -8.090 0.001

SrOH+ 5.358e-012 4.852e-012 -11.271 -11.314 -0.043

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -0.65 10.96 11.61 Al(OH)3

Albite -2.80 -21.60 -18.80 NaAlSi3O8

Alunite -0.52 -0.37 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.18 -6.51 -4.33 CaSO4

Anorthite -2.58 -22.65 -20.07 CaAl2Si2O8

Aragonite -0.18 -8.45 -8.27 CaCO3

Barite 0.11 -10.07 -10.18 BaSO4

Ca-Montmorillonite 3.73 -43.09 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite -0.03 -8.45 -8.42 CaCO3

Celestite -2.18 -8.80 -6.62 SrSO4

Chalcedony -0.30 -3.99 -3.70 SiO2

Chlorite(14A) -8.44 64.60 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -8.95 24.80 33.75 Mg3Si2O5(OH)4

CO2(g) -1.60 -2.92 -1.31 CO2

Dolomite -0.52 -17.32 -16.80 CaMg(CO3)2

Gibbsite 2.15 10.96 8.81 Al(OH)3

Gypsum -1.92 -6.51 -4.59 CaSO4:2H2O

H2(g) -39.57 -42.67 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.41 -7.86 1.55 NaCl

Illite 2.27 -39.68 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -1.00 -22.52 -21.52 KAlSi3O8

K-mica 8.85 23.38 14.53 KAl3Si3O10(OH)2

Kaolinite 5.42 13.94 8.52 Al2Si2O5(OH)4

O2(g) -8.29 -11.08 -2.79 O2

Quartz 0.17 -3.99 -4.16 SiO2

Sepiolite -6.21 9.88 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.78 9.88 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.18 -3.99 -2.81 SiO2

Strontianite -1.46 -10.74 -9.28 SrCO3

Talc -6.01 16.82 22.82 Mg3Si4O10(OH)2

Witherite -3.40 -12.01 -8.61 BaCO3

Initial solution 16. 07-10-28

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 9.271e-006 9.271e-006

Alkalinity 6.133e-003 6.133e-003

B 3.887e-006 3.887e-006

Ba 6.848e-007 6.848e-007

Ca 2.516e-003 2.516e-003

Cl 8.382e-005 8.382e-005

K 2.815e-005 2.815e-005

Li 4.326e-006 4.326e-006

Mg 9.630e-004 9.630e-004

N(5) 1.572e-006 1.572e-006

Na 2.333e-004 2.333e-004

S(6) 4.615e-004 4.615e-004

Si 1.116e-004 1.116e-004

Sr 1.359e-005 1.359e-005

----------------------------Description of solution----------------------------

pH = 7.091 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 474

Density (g/cm3) = 0.99985

Activity of water = 1.000

Ionic strength = 1.048e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.275e-003

Total CO2 (mol/kg) = 7.275e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = 1.398e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 1.02

Iterations = 11

Total H = 1.110190e+002

Total O = 5.552920e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

H+ 8.885e-008 8.116e-008 -7.051 -7.091 -0.039

OH- 5.205e-008 4.684e-008 -7.284 -7.329 -0.046

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 9.271e-006

Al(OH)4- 8.302e-006 7.488e-006 -5.081 -5.126 -0.045

Al(OH)2+ 5.796e-007 5.227e-007 -6.237 -6.282 -0.045

Al(OH)3 3.628e-007 3.637e-007 -6.440 -6.439 0.001

AlOH+2 2.523e-008 1.670e-008 -7.598 -7.777 -0.179

Al+3 6.868e-010 3.040e-010 -9.163 -9.517 -0.354

AlSO4+ 2.222e-010 2.004e-010 -9.653 -9.698 -0.045

Al(SO4)2- 1.625e-012 1.466e-012 -11.789 -11.834 -0.045

AlHSO4+2 1.999e-018 1.323e-018 -17.699 -17.878 -0.179

B 3.887e-006

H3BO3 3.863e-006 3.873e-006 -5.413 -5.412 0.001

H2BO3- 2.423e-008 2.186e-008 -7.616 -7.660 -0.045

Ba 6.848e-007

Ba+2 6.177e-007 4.126e-007 -6.209 -6.385 -0.175

BaSO4 5.056e-008 5.068e-008 -7.296 -7.295 0.001

BaHCO3+ 1.616e-008 1.458e-008 -7.792 -7.836 -0.045

BaCO3 3.916e-010 3.925e-010 -9.407 -9.406 0.001

BaOH+ 1.909e-013 1.722e-013 -12.719 -12.764 -0.045

C(4) 7.275e-003

HCO3- 5.942e-003 5.377e-003 -2.226 -2.269 -0.043

CO2 1.187e-003 1.190e-003 -2.925 -2.924 0.001

CaHCO3+ 9.415e-005 8.521e-005 -4.026 -4.070 -0.043

MgHCO3+ 4.063e-005 3.665e-005 -4.391 -4.436 -0.045

CaCO3 5.154e-006 5.166e-006 -5.288 -5.287 0.001

CO3-2 3.493e-006 2.343e-006 -5.457 -5.630 -0.173

MgCO3 1.122e-006 1.125e-006 -5.950 -5.949 0.001

NaHCO3 6.330e-007 6.345e-007 -6.199 -6.198 0.001

SrHCO3+ 5.148e-007 4.659e-007 -6.288 -6.332 -0.043

BaHCO3+ 1.616e-008 1.458e-008 -7.792 -7.836 -0.045

SrCO3 8.944e-009 8.965e-009 -8.048 -8.047 0.001

NaCO3- 5.403e-009 4.873e-009 -8.267 -8.312 -0.045

BaCO3 3.916e-010 3.925e-010 -9.407 -9.406 0.001

Ca 2.516e-003

Ca+2 2.349e-003 1.575e-003 -2.629 -2.803 -0.174

CaHCO3+ 9.415e-005 8.521e-005 -4.026 -4.070 -0.043

CaSO4 6.836e-005 6.853e-005 -4.165 -4.164 0.001

CaCO3 5.154e-006 5.166e-006 -5.288 -5.287 0.001

CaOH+ 3.570e-009 3.220e-009 -8.447 -8.492 -0.045

CaHSO4+ 3.167e-011 2.857e-011 -10.499 -10.544 -0.045

Cl 8.382e-005

Cl- 8.382e-005 7.546e-005 -4.077 -4.122 -0.046

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -42.678 -42.677 0.001

K 2.815e-005

K+ 2.811e-005 2.530e-005 -4.551 -4.597 -0.046

KSO4- 3.885e-008 3.504e-008 -7.411 -7.455 -0.045

KOH 1.078e-012 1.081e-012 -11.967 -11.966 0.001

Li 4.326e-006

Li+ 4.321e-006 3.917e-006 -5.364 -5.407 -0.043

LiSO4- 4.647e-009 4.191e-009 -8.333 -8.378 -0.045

LiOH 1.103e-012 1.106e-012 -11.957 -11.956 0.001

Mg 9.630e-004

Mg+2 8.961e-004 6.049e-004 -3.048 -3.218 -0.171

MgHCO3+ 4.063e-005 3.665e-005 -4.391 -4.436 -0.045

MgSO4 2.512e-005 2.518e-005 -4.600 -4.599 0.001

MgCO3 1.122e-006 1.125e-006 -5.950 -5.949 0.001

MgOH+ 9.699e-009 8.748e-009 -8.013 -8.058 -0.045

N(5) 1.572e-006

NO3- 1.572e-006 1.412e-006 -5.804 -5.850 -0.046

Na 2.333e-004

Na+ 2.324e-004 2.098e-004 -3.634 -3.678 -0.044

NaHCO3 6.330e-007 6.345e-007 -6.199 -6.198 0.001

NaSO4- 2.640e-007 2.381e-007 -6.578 -6.623 -0.045

NaCO3- 5.403e-009 4.873e-009 -8.267 -8.312 -0.045

NaOH 1.704e-011 1.708e-011 -10.769 -10.768 0.001

O(0) 1.735e-011

O2 8.674e-012 8.695e-012 -11.062 -11.061 0.001

S(6) 4.615e-004

SO4-2 3.673e-004 2.451e-004 -3.435 -3.611 -0.176

CaSO4 6.836e-005 6.853e-005 -4.165 -4.164 0.001

MgSO4 2.512e-005 2.518e-005 -4.600 -4.599 0.001

SrSO4 3.515e-007 3.523e-007 -6.454 -6.453 0.001

NaSO4- 2.640e-007 2.381e-007 -6.578 -6.623 -0.045

BaSO4 5.056e-008 5.068e-008 -7.296 -7.295 0.001

KSO4- 3.885e-008 3.504e-008 -7.411 -7.455 -0.045

LiSO4- 4.647e-009 4.191e-009 -8.333 -8.378 -0.045

HSO4- 1.673e-009 1.509e-009 -8.777 -8.821 -0.045

AlSO4+ 2.222e-010 2.004e-010 -9.653 -9.698 -0.045

CaHSO4+ 3.167e-011 2.857e-011 -10.499 -10.544 -0.045

Al(SO4)2- 1.625e-012 1.466e-012 -11.789 -11.834 -0.045

AlHSO4+2 1.999e-018 1.323e-018 -17.699 -17.878 -0.179

Si 1.116e-004

H4SiO4 1.114e-004 1.117e-004 -3.953 -3.952 0.001

H3SiO4- 1.432e-007 1.291e-007 -6.844 -6.889 -0.045

H2SiO4-2 7.064e-014 4.675e-014 -13.151 -13.330 -0.179

Sr 1.359e-005

Sr+2 1.271e-005 8.542e-006 -4.896 -5.068 -0.173

SrHCO3+ 5.148e-007 4.659e-007 -6.288 -6.332 -0.043

SrSO4 3.515e-007 3.523e-007 -6.454 -6.453 0.001

SrCO3 8.944e-009 8.965e-009 -8.048 -8.047 0.001

SrOH+ 5.970e-012 5.397e-012 -11.224 -11.268 -0.044

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) 0.14 11.75 11.61 Al(OH)3

Albite -1.86 -20.66 -18.80 NaAlSi3O8

Alunite 2.03 2.17 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.08 -6.41 -4.33 CaSO4

Anorthite -0.89 -20.96 -20.07 CaAl2Si2O8

Aragonite -0.16 -8.43 -8.27 CaCO3

Barite 0.19 -10.00 -10.18 BaSO4

Ca-Montmorillonite 5.73 -41.09 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite -0.01 -8.43 -8.42 CaCO3

Celestite -2.06 -8.68 -6.62 SrSO4

Chalcedony -0.26 -3.95 -3.70 SiO2

Chlorite(14A) -6.57 66.47 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -8.76 24.98 33.75 Mg3Si2O5(OH)4

CO2(g) -1.61 -2.92 -1.31 CO2

Dolomite -0.48 -17.28 -16.80 CaMg(CO3)2

Gibbsite 2.94 11.75 8.81 Al(OH)3

Gypsum -1.83 -6.41 -4.59 CaSO4:2H2O

H2(g) -39.58 -42.68 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.35 -7.80 1.55 NaCl

Illite 4.26 -37.69 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -0.06 -21.58 -21.52 KAlSi3O8

K-mica 11.37 25.90 14.53 KAl3Si3O10(OH)2

Kaolinite 7.09 15.61 8.52 Al2Si2O5(OH)4

O2(g) -8.27 -11.06 -2.79 O2

Quartz 0.21 -3.95 -4.16 SiO2

Sepiolite -6.02 10.07 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.59 10.07 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.14 -3.95 -2.81 SiO2

Strontianite -1.42 -10.70 -9.28 SrCO3

Talc -5.74 17.08 22.82 Mg3Si4O10(OH)2

Witherite -3.40 -12.01 -8.61 BaCO3

Initial solution 17. 07-11-18

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 6.297e-003 6.297e-003

B 3.795e-006 3.795e-006

Ba 6.630e-007 6.630e-007

Ca 2.484e-003 2.484e-003

Cl 7.620e-005 7.620e-005

K 2.508e-005 2.508e-005

Li 4.326e-006 4.326e-006

Mg 9.672e-004 9.672e-004

Na 2.368e-004 2.368e-004

S(6) 4.617e-004 4.617e-004

Si 9.992e-005 9.992e-005

Sr 1.359e-005 1.359e-005

----------------------------Description of solution----------------------------

pH = 7.157 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 478

Density (g/cm3) = 0.99985

Activity of water = 1.000

Ionic strength = 1.051e-002

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.336e-003

Total CO2 (mol/kg) = 7.336e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -9.948e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.72

Iterations = 9

Total H = 1.110191e+002

Total O = 5.552943e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

H+ 7.620e-008 6.960e-008 -7.118 -7.157 -0.039

OH- 6.071e-008 5.463e-008 -7.217 -7.263 -0.046

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 3.795e-006

H3BO3 3.767e-006 3.777e-006 -5.424 -5.423 0.001

H2BO3- 2.756e-008 2.485e-008 -7.560 -7.605 -0.045

Ba 6.630e-007

Ba+2 5.974e-007 3.988e-007 -6.224 -6.399 -0.175

BaSO4 4.898e-008 4.910e-008 -7.310 -7.309 0.001

BaHCO3+ 1.613e-008 1.455e-008 -7.792 -7.837 -0.045

BaCO3 4.557e-010 4.568e-010 -9.341 -9.340 0.001

BaOH+ 2.153e-013 1.941e-013 -12.667 -12.712 -0.045

C(4) 7.336e-003

HCO3- 6.134e-003 5.551e-003 -2.212 -2.256 -0.043

CO2 1.051e-003 1.054e-003 -2.978 -2.977 0.001

CaHCO3+ 9.574e-005 8.664e-005 -4.019 -4.062 -0.043

MgHCO3+ 4.204e-005 3.792e-005 -4.376 -4.421 -0.045

CaCO3 6.111e-006 6.126e-006 -5.214 -5.213 0.001

CO3-2 4.206e-006 2.821e-006 -5.376 -5.550 -0.174

MgCO3 1.354e-006 1.357e-006 -5.868 -5.867 0.001

NaHCO3 6.630e-007 6.646e-007 -6.178 -6.177 0.001

SrHCO3+ 5.305e-007 4.801e-007 -6.275 -6.319 -0.043

BaHCO3+ 1.613e-008 1.455e-008 -7.792 -7.837 -0.045

SrCO3 1.075e-008 1.077e-008 -7.969 -7.968 0.001

NaCO3- 6.601e-009 5.953e-009 -8.180 -8.225 -0.045

BaCO3 4.557e-010 4.568e-010 -9.341 -9.340 0.001

Ca 2.484e-003

Ca+2 2.315e-003 1.551e-003 -2.636 -2.809 -0.174

CaHCO3+ 9.574e-005 8.664e-005 -4.019 -4.062 -0.043

CaSO4 6.749e-005 6.765e-005 -4.171 -4.170 0.001

CaCO3 6.111e-006 6.126e-006 -5.214 -5.213 0.001

CaOH+ 4.101e-009 3.699e-009 -8.387 -8.432 -0.045

CaHSO4+ 2.682e-011 2.418e-011 -10.572 -10.616 -0.045

Cl 7.620e-005

Cl- 7.620e-005 6.859e-005 -4.118 -4.164 -0.046

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -42.812 -42.811 0.001

K 2.508e-005

K+ 2.504e-005 2.254e-005 -4.601 -4.647 -0.046

KSO4- 3.468e-008 3.128e-008 -7.460 -7.505 -0.045

KOH 1.120e-012 1.123e-012 -11.951 -11.950 0.001

Li 4.326e-006

Li+ 4.321e-006 3.917e-006 -5.364 -5.407 -0.043

LiSO4- 4.657e-009 4.200e-009 -8.332 -8.377 -0.045

LiOH 1.286e-012 1.289e-012 -11.891 -11.890 0.001

Mg 9.672e-004

Mg+2 8.985e-004 6.062e-004 -3.046 -3.217 -0.171

MgHCO3+ 4.204e-005 3.792e-005 -4.376 -4.421 -0.045

MgSO4 2.523e-005 2.529e-005 -4.598 -4.597 0.001

MgCO3 1.354e-006 1.357e-006 -5.868 -5.867 0.001

MgOH+ 1.134e-008 1.022e-008 -7.946 -7.990 -0.045

Na 2.368e-004

Na+ 2.358e-004 2.129e-004 -3.627 -3.672 -0.044

NaHCO3 6.630e-007 6.646e-007 -6.178 -6.177 0.001

NaSO4- 2.685e-007 2.421e-007 -6.571 -6.616 -0.045

NaCO3- 6.601e-009 5.953e-009 -8.180 -8.225 -0.045

NaOH 2.016e-011 2.021e-011 -10.696 -10.694 0.001

O(0) 3.208e-011

O2 1.604e-011 1.608e-011 -10.795 -10.794 0.001

S(6) 4.617e-004

SO4-2 3.683e-004 2.456e-004 -3.434 -3.610 -0.176

CaSO4 6.749e-005 6.765e-005 -4.171 -4.170 0.001

MgSO4 2.523e-005 2.529e-005 -4.598 -4.597 0.001

SrSO4 3.516e-007 3.524e-007 -6.454 -6.453 0.001

NaSO4- 2.685e-007 2.421e-007 -6.571 -6.616 -0.045

BaSO4 4.898e-008 4.910e-008 -7.310 -7.309 0.001

KSO4- 3.468e-008 3.128e-008 -7.460 -7.505 -0.045

LiSO4- 4.657e-009 4.200e-009 -8.332 -8.377 -0.045

HSO4- 1.438e-009 1.297e-009 -8.842 -8.887 -0.045

CaHSO4+ 2.682e-011 2.418e-011 -10.572 -10.616 -0.045

Si 9.992e-005

H4SiO4 9.977e-005 1.000e-004 -4.001 -4.000 0.001

H3SiO4- 1.495e-007 1.348e-007 -6.825 -6.870 -0.045

H2SiO4-2 8.605e-014 5.692e-014 -13.065 -13.245 -0.180

Sr 1.359e-005

Sr+2 1.270e-005 8.526e-006 -4.896 -5.069 -0.173

SrHCO3+ 5.305e-007 4.801e-007 -6.275 -6.319 -0.043

SrSO4 3.516e-007 3.524e-007 -6.454 -6.453 0.001

SrCO3 1.075e-008 1.077e-008 -7.969 -7.968 0.001

SrOH+ 6.950e-012 6.282e-012 -11.158 -11.202 -0.044

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.08 -6.42 -4.33 CaSO4

Aragonite -0.09 -8.36 -8.27 CaCO3

Barite 0.17 -10.01 -10.18 BaSO4

Calcite 0.06 -8.36 -8.42 CaCO3

Celestite -2.06 -8.68 -6.62 SrSO4

Chalcedony -0.30 -4.00 -3.70 SiO2

Chrysotile -8.46 25.29 33.75 Mg3Si2O5(OH)4

CO2(g) -1.66 -2.98 -1.31 CO2

Dolomite -0.33 -17.13 -16.80 CaMg(CO3)2

Gypsum -1.83 -6.42 -4.59 CaSO4:2H2O

H2(g) -39.71 -42.81 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.39 -7.84 1.55 NaCl

O2(g) -8.00 -10.79 -2.79 O2

Quartz 0.16 -4.00 -4.16 SiO2

Sepiolite -5.89 10.20 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.46 10.20 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.19 -4.00 -2.81 SiO2

Strontianite -1.34 -10.62 -9.28 SrCO3

Talc -5.53 17.29 22.82 Mg3Si4O10(OH)2

Witherite -3.34 -11.95 -8.61 BaCO3

Initial solution 18. 08-4-6

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 2.262e-006 2.262e-006

Alkalinity 5.706e-003 5.706e-003

B 1.944e-006 1.944e-006

Ba 6.411e-007 6.411e-007

Ca 2.182e-003 2.182e-003

Cl 6.293e-005 6.293e-005

K 2.175e-005 2.175e-005

Li 3.749e-006 3.749e-006

Mg 7.654e-004 7.654e-004

Na 1.836e-004 1.836e-004

S(6) 2.075e-004 2.075e-004

Si 7.959e-005 7.959e-005

Sr 9.021e-006 9.021e-006

----------------------------Description of solution----------------------------

pH = 7.865 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 407

Density (g/cm3) = 0.99978

Activity of water = 1.000

Ionic strength = 8.866e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 5.832e-003

Total CO2 (mol/kg) = 5.832e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -5.426e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.46

Iterations = 11

Total H = 1.110184e+002

Total O = 5.552469e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.069e-007 2.783e-007 -6.513 -6.555 -0.042

H+ 1.487e-008 1.366e-008 -7.828 -7.865 -0.037

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 2.262e-006

Al(OH)4- 2.241e-006 2.036e-006 -5.650 -5.691 -0.042

Al(OH)3 1.661e-008 1.664e-008 -7.780 -7.779 0.001

Al(OH)2+ 4.430e-009 4.025e-009 -8.354 -8.395 -0.042

AlOH+2 3.176e-011 2.164e-011 -10.498 -10.665 -0.167

Al+3 1.423e-013 6.631e-014 -12.847 -13.178 -0.332

AlSO4+ 2.270e-014 2.062e-014 -13.644 -13.686 -0.042

Al(SO4)2- 7.832e-017 7.115e-017 -16.106 -16.148 -0.042

AlHSO4+2 3.363e-023 2.291e-023 -22.473 -22.640 -0.167

B 1.944e-006

H3BO3 1.874e-006 1.878e-006 -5.727 -5.726 0.001

H2BO3- 6.932e-008 6.298e-008 -7.159 -7.201 -0.042

Ba 6.411e-007

Ba+2 6.001e-007 4.122e-007 -6.222 -6.385 -0.163

BaSO4 2.384e-008 2.389e-008 -7.623 -7.622 0.001

BaHCO3+ 1.491e-008 1.354e-008 -7.827 -7.868 -0.042

BaCO3 2.162e-009 2.167e-009 -8.665 -8.664 0.001

BaOH+ 1.125e-012 1.022e-012 -11.949 -11.990 -0.042

C(4) 5.832e-003

HCO3- 5.487e-003 5.000e-003 -2.261 -2.301 -0.040

CO2 1.859e-004 1.863e-004 -3.731 -3.730 0.001

CaHCO3+ 7.797e-005 7.105e-005 -4.108 -4.148 -0.040

MgHCO3+ 3.093e-005 2.810e-005 -4.510 -4.551 -0.042

CaCO3 2.554e-005 2.560e-005 -4.593 -4.592 0.001

CO3-2 1.878e-005 1.295e-005 -4.726 -4.888 -0.161

MgCO3 5.114e-006 5.125e-006 -5.291 -5.290 0.001

NaHCO3 4.672e-007 4.681e-007 -6.331 -6.330 0.001

SrHCO3+ 3.283e-007 2.992e-007 -6.484 -6.524 -0.040

SrCO3 3.413e-008 3.420e-008 -7.467 -7.466 0.001

NaCO3- 2.351e-008 2.136e-008 -7.629 -7.670 -0.042

BaHCO3+ 1.491e-008 1.354e-008 -7.827 -7.868 -0.042

BaCO3 2.162e-009 2.167e-009 -8.665 -8.664 0.001

Ca 2.182e-003

Ca+2 2.049e-003 1.412e-003 -2.688 -2.850 -0.162

CaHCO3+ 7.797e-005 7.105e-005 -4.108 -4.148 -0.040

CaSO4 2.894e-005 2.899e-005 -4.539 -4.538 0.001

CaCO3 2.554e-005 2.560e-005 -4.593 -4.592 0.001

CaOH+ 1.888e-008 1.716e-008 -7.724 -7.766 -0.042

CaHSO4+ 2.239e-012 2.034e-012 -11.650 -11.692 -0.042

Cl 6.293e-005

Cl- 6.293e-005 5.708e-005 -4.201 -4.243 -0.042

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -44.226 -44.225 0.001

K 2.175e-005

K+ 2.173e-005 1.972e-005 -4.663 -4.705 -0.042

KSO4- 1.418e-008 1.288e-008 -7.848 -7.890 -0.042

KOH 4.994e-012 5.004e-012 -11.302 -11.301 0.001

Li 3.749e-006

Li+ 3.747e-006 3.419e-006 -5.426 -5.466 -0.040

LiSO4- 1.900e-009 1.726e-009 -8.721 -8.763 -0.042

LiOH 5.722e-012 5.734e-012 -11.242 -11.242 0.001

Mg 7.654e-004

Mg+2 7.196e-004 4.987e-004 -3.143 -3.302 -0.159

MgHCO3+ 3.093e-005 2.810e-005 -4.510 -4.551 -0.042

MgSO4 9.777e-006 9.797e-006 -5.010 -5.009 0.001

MgCO3 5.114e-006 5.125e-006 -5.291 -5.290 0.001

MgOH+ 4.717e-008 4.286e-008 -7.326 -7.368 -0.042

Na 1.836e-004

Na+ 1.831e-004 1.665e-004 -3.737 -3.779 -0.041

NaHCO3 4.672e-007 4.681e-007 -6.331 -6.330 0.001

NaSO4- 9.811e-008 8.913e-008 -7.008 -7.050 -0.042

NaCO3- 2.351e-008 2.136e-008 -7.629 -7.670 -0.042

NaOH 8.035e-011 8.052e-011 -10.095 -10.094 0.001

O(0) 2.163e-008

O2 1.082e-008 1.084e-008 -7.966 -7.965 0.001

S(6) 2.075e-004

SO4-2 1.685e-004 1.156e-004 -3.773 -3.937 -0.163

CaSO4 2.894e-005 2.899e-005 -4.539 -4.538 0.001

MgSO4 9.777e-006 9.797e-006 -5.010 -5.009 0.001

SrSO4 1.146e-007 1.148e-007 -6.941 -6.940 0.001

NaSO4- 9.811e-008 8.913e-008 -7.008 -7.050 -0.042

BaSO4 2.384e-008 2.389e-008 -7.623 -7.622 0.001

KSO4- 1.418e-008 1.288e-008 -7.848 -7.890 -0.042

LiSO4- 1.900e-009 1.726e-009 -8.721 -8.763 -0.042

HSO4- 1.319e-010 1.198e-010 -9.880 -9.922 -0.042

CaHSO4+ 2.239e-012 2.034e-012 -11.650 -11.692 -0.042

AlSO4+ 2.270e-014 2.062e-014 -13.644 -13.686 -0.042

Al(SO4)2- 7.832e-017 7.115e-017 -16.106 -16.148 -0.042

AlHSO4+2 3.363e-023 2.291e-023 -22.473 -22.640 -0.167

Si 7.959e-005

H4SiO4 7.900e-005 7.916e-005 -4.102 -4.102 0.001

H3SiO4- 5.985e-007 5.437e-007 -6.223 -6.265 -0.042

H2SiO4-2 1.717e-012 1.170e-012 -11.765 -11.932 -0.167

Sr 9.021e-006

Sr+2 8.544e-006 5.898e-006 -5.068 -5.229 -0.161

SrHCO3+ 3.283e-007 2.992e-007 -6.484 -6.524 -0.040

SrSO4 1.146e-007 1.148e-007 -6.941 -6.940 0.001

SrCO3 3.413e-008 3.420e-008 -7.467 -7.466 0.001

SrOH+ 2.432e-011 2.214e-011 -10.614 -10.655 -0.041

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -1.20 10.42 11.61 Al(OH)3

Albite -2.98 -21.77 -18.80 NaAlSi3O8

Alunite -5.07 -4.93 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.45 -6.79 -4.33 CaSO4

Anorthite -2.37 -22.44 -20.07 CaAl2Si2O8

Aragonite 0.53 -7.74 -8.27 CaCO3

Barite -0.14 -10.32 -10.18 BaSO4

Ca-Montmorillonite 2.31 -44.51 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.68 -7.74 -8.42 CaCO3

Celestite -2.54 -9.17 -6.62 SrSO4

Chalcedony -0.40 -4.10 -3.70 SiO2

Chlorite(14A) -2.38 70.66 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -4.67 29.08 33.75 Mg3Si2O5(OH)4

CO2(g) -2.42 -3.73 -1.31 CO2

Dolomite 0.87 -15.93 -16.80 CaMg(CO3)2

Gibbsite 1.60 10.42 8.81 Al(OH)3

Gypsum -2.20 -6.79 -4.59 CaSO4:2H2O

H2(g) -41.13 -44.23 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.58 -8.02 1.55 NaCl

Illite 1.42 -40.53 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -1.18 -22.70 -21.52 KAlSi3O8

K-mica 7.57 22.10 14.53 KAl3Si3O10(OH)2

Kaolinite 4.11 12.63 8.52 Al2Si2O5(OH)4

O2(g) -5.17 -7.97 -2.79 O2

Quartz 0.06 -4.10 -4.16 SiO2

Sepiolite -3.54 12.55 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -6.11 12.55 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.29 -4.10 -2.81 SiO2

Strontianite -0.84 -10.12 -9.28 SrCO3

Talc -1.95 20.88 22.82 Mg3Si4O10(OH)2

Witherite -2.66 -11.27 -8.61 BaCO3

Initial solution 19. 08-5-20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 5.936e-003 5.936e-003

B 2.406e-006 2.406e-006

Ba 6.484e-007 6.484e-007

Ca 2.294e-003 2.294e-003

Cl 8.353e-005 8.353e-005

K 2.303e-005 2.303e-005

Li 4.181e-006 4.181e-006

Mg 8.478e-004 8.478e-004

Na 2.019e-004 2.019e-004

S(6) 2.512e-004 2.512e-004

Si 8.742e-005 8.742e-005

Sr 1.119e-005 1.119e-005

----------------------------Description of solution----------------------------

pH = 7.600 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 432

Density (g/cm3) = 0.99981

Activity of water = 1.000

Ionic strength = 9.451e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.263e-003

Total CO2 (mol/kg) = 6.263e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = 1.494e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.12

Iterations = 9

Total H = 1.110187e+002

Total O = 5.552601e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.674e-007 1.514e-007 -6.776 -6.820 -0.044

H+ 2.740e-008 2.512e-008 -7.562 -7.600 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 2.406e-006

H3BO3 2.359e-006 2.364e-006 -5.627 -5.626 0.001

H2BO3- 4.758e-008 4.311e-008 -7.323 -7.365 -0.043

Ba 6.484e-007

Ba+2 6.034e-007 4.101e-007 -6.219 -6.387 -0.168

BaSO4 2.818e-008 2.824e-008 -7.550 -7.549 0.001

BaHCO3+ 1.556e-008 1.409e-008 -7.808 -7.851 -0.043

BaCO3 1.224e-009 1.226e-009 -8.912 -8.911 0.001

BaOH+ 6.106e-013 5.532e-013 -12.214 -12.257 -0.043

C(4) 6.263e-003

HCO3- 5.755e-003 5.231e-003 -2.240 -2.281 -0.041

CO2 3.575e-004 3.583e-004 -3.447 -3.446 0.001

CaHCO3+ 8.523e-005 7.746e-005 -4.069 -4.111 -0.041

MgHCO3+ 3.554e-005 3.220e-005 -4.449 -4.492 -0.043

CaCO3 1.514e-005 1.518e-005 -4.820 -4.819 0.001

CO3-2 1.079e-005 7.366e-006 -4.967 -5.133 -0.166

MgCO3 3.187e-006 3.194e-006 -5.497 -5.496 0.001

NaHCO3 5.358e-007 5.369e-007 -6.271 -6.270 0.001

SrHCO3+ 4.220e-007 3.835e-007 -6.375 -6.416 -0.041

SrCO3 2.379e-008 2.385e-008 -7.624 -7.623 0.001

BaHCO3+ 1.556e-008 1.409e-008 -7.808 -7.851 -0.043

NaCO3- 1.471e-008 1.333e-008 -7.832 -7.875 -0.043

BaCO3 1.224e-009 1.226e-009 -8.912 -8.911 0.001

Ca 2.294e-003

Ca+2 2.158e-003 1.472e-003 -2.666 -2.832 -0.166

CaHCO3+ 8.523e-005 7.746e-005 -4.069 -4.111 -0.041

CaSO4 3.582e-005 3.590e-005 -4.446 -4.445 0.001

CaCO3 1.514e-005 1.518e-005 -4.820 -4.819 0.001

CaOH+ 1.073e-008 9.724e-009 -7.969 -8.012 -0.043

CaHSO4+ 5.112e-012 4.632e-012 -11.291 -11.334 -0.043

Cl 8.353e-005

Cl- 8.353e-005 7.556e-005 -4.078 -4.122 -0.044

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.697 -43.696 0.001

K 2.303e-005

K+ 2.301e-005 2.081e-005 -4.638 -4.682 -0.044

KSO4- 1.783e-008 1.615e-008 -7.749 -7.792 -0.043

KOH 2.867e-012 2.873e-012 -11.543 -11.542 0.001

Li 4.181e-006

Li+ 4.179e-006 3.804e-006 -5.379 -5.420 -0.041

LiSO4- 2.518e-009 2.281e-009 -8.599 -8.642 -0.043

LiOH 3.462e-012 3.469e-012 -11.461 -11.460 0.001

Mg 8.478e-004

Mg+2 7.963e-004 5.464e-004 -3.099 -3.262 -0.164

MgHCO3+ 3.554e-005 3.220e-005 -4.449 -4.492 -0.043

MgSO4 1.273e-005 1.275e-005 -4.895 -4.894 0.001

MgCO3 3.187e-006 3.194e-006 -5.497 -5.496 0.001

MgOH+ 2.818e-008 2.554e-008 -7.550 -7.593 -0.043

Na 2.019e-004

Na+ 2.013e-004 1.825e-004 -3.696 -3.739 -0.042

NaHCO3 5.358e-007 5.369e-007 -6.271 -6.270 0.001

NaSO4- 1.282e-007 1.161e-007 -6.892 -6.935 -0.043

NaCO3- 1.471e-008 1.333e-008 -7.832 -7.875 -0.043

NaOH 4.790e-011 4.801e-011 -10.320 -10.319 0.001

O(0) 1.892e-009

O2 9.459e-010 9.480e-010 -9.024 -9.023 0.001

S(6) 2.512e-004

SO4-2 2.023e-004 1.374e-004 -3.694 -3.862 -0.168

CaSO4 3.582e-005 3.590e-005 -4.446 -4.445 0.001

MgSO4 1.273e-005 1.275e-005 -4.895 -4.894 0.001

SrSO4 1.668e-007 1.671e-007 -6.778 -6.777 0.001

NaSO4- 1.282e-007 1.161e-007 -6.892 -6.935 -0.043

BaSO4 2.818e-008 2.824e-008 -7.550 -7.549 0.001

KSO4- 1.783e-008 1.615e-008 -7.749 -7.792 -0.043

LiSO4- 2.518e-009 2.281e-009 -8.599 -8.642 -0.043

HSO4- 2.889e-010 2.617e-010 -9.539 -9.582 -0.043

CaHSO4+ 5.112e-012 4.632e-012 -11.291 -11.334 -0.043

Si 8.742e-005

H4SiO4 8.706e-005 8.725e-005 -4.060 -4.059 0.001

H3SiO4- 3.598e-007 3.259e-007 -6.444 -6.487 -0.043

H2SiO4-2 5.658e-013 3.813e-013 -12.247 -12.419 -0.171

Sr 1.119e-005

Sr+2 1.058e-005 7.228e-006 -4.976 -5.141 -0.165

SrHCO3+ 4.220e-007 3.835e-007 -6.375 -6.416 -0.041

SrSO4 1.668e-007 1.671e-007 -6.778 -6.777 0.001

SrCO3 2.379e-008 2.385e-008 -7.624 -7.623 0.001

SrOH+ 1.625e-011 1.476e-011 -10.789 -10.831 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.36 -6.69 -4.33 CaSO4

Aragonite 0.30 -7.96 -8.27 CaCO3

Barite -0.07 -10.25 -10.18 BaSO4

Calcite 0.46 -7.96 -8.42 CaCO3

Celestite -2.38 -9.00 -6.62 SrSO4

Chalcedony -0.36 -4.06 -3.70 SiO2

Chrysotile -6.05 27.69 33.75 Mg3Si2O5(OH)4

CO2(g) -2.13 -3.45 -1.31 CO2

Dolomite 0.44 -16.36 -16.80 CaMg(CO3)2

Gypsum -2.11 -6.69 -4.59 CaSO4:2H2O

H2(g) -40.60 -43.70 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.41 -7.86 1.55 NaCl

O2(g) -6.23 -9.02 -2.79 O2

Quartz 0.11 -4.06 -4.16 SiO2

Sepiolite -4.39 11.70 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -6.96 11.70 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.24 -4.06 -2.81 SiO2

Strontianite -0.99 -10.27 -9.28 SrCO3

Talc -3.25 19.58 22.82 Mg3Si4O10(OH)2

Witherite -2.91 -11.52 -8.61 BaCO3

Initial solution 20. 08-6-21

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 6.247e-003 6.247e-003

B 2.962e-006 2.962e-006

Ba 6.411e-007 6.411e-007

Ca 2.314e-003 2.314e-003

Cl 8.918e-005 8.918e-005

K 2.482e-005 2.482e-005

Li 4.758e-006 4.758e-006

Mg 8.972e-004 8.972e-004

N(5) 6.000e-006 6.000e-006

Na 2.224e-004 2.224e-004

S(6) 2.398e-004 2.398e-004

Si 9.425e-005 9.425e-005

Sr 1.245e-005 1.245e-005

----------------------------Description of solution----------------------------

pH = 7.384 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 447

Density (g/cm3) = 0.99982

Activity of water = 1.000

Ionic strength = 9.747e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.849e-003

Total CO2 (mol/kg) = 6.849e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -1.213e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.93

Iterations = 9

Total H = 1.110190e+002

Total O = 5.552751e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.019e-007 9.197e-008 -6.992 -7.036 -0.044

H+ 4.514e-008 4.134e-008 -7.345 -7.384 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 2.962e-006

H3BO3 2.926e-006 2.932e-006 -5.534 -5.533 0.001

H2BO3- 3.591e-008 3.249e-008 -7.445 -7.488 -0.043

Ba 6.411e-007

Ba+2 5.978e-007 4.042e-007 -6.223 -6.393 -0.170

BaSO4 2.630e-008 2.636e-008 -7.580 -7.579 0.001

BaHCO3+ 1.620e-008 1.465e-008 -7.791 -7.834 -0.043

BaCO3 7.730e-010 7.748e-010 -9.112 -9.111 0.001

BaOH+ 3.662e-013 3.313e-013 -12.436 -12.480 -0.043

C(4) 6.849e-003

HCO3- 6.078e-003 5.518e-003 -2.216 -2.258 -0.042

CO2 6.206e-004 6.220e-004 -3.207 -3.206 0.001

CaHCO3+ 9.047e-005 8.212e-005 -4.044 -4.086 -0.042

MgHCO3+ 3.954e-005 3.578e-005 -4.403 -4.446 -0.043

CaCO3 9.755e-006 9.777e-006 -5.011 -5.010 0.001

CO3-2 6.952e-006 4.721e-006 -5.158 -5.326 -0.168

MgCO3 2.151e-006 2.156e-006 -5.667 -5.666 0.001

NaHCO3 6.215e-007 6.229e-007 -6.207 -6.206 0.001

SrHCO3+ 4.931e-007 4.476e-007 -6.307 -6.349 -0.042

SrCO3 1.687e-008 1.691e-008 -7.773 -7.772 0.001

BaHCO3+ 1.620e-008 1.465e-008 -7.791 -7.834 -0.043

NaCO3- 1.038e-008 9.393e-009 -7.984 -8.027 -0.043

BaCO3 7.730e-010 7.748e-010 -9.112 -9.111 0.001

Ca 2.314e-003

Ca+2 2.180e-003 1.479e-003 -2.662 -2.830 -0.168

CaHCO3+ 9.047e-005 8.212e-005 -4.044 -4.086 -0.042

CaSO4 3.410e-005 3.418e-005 -4.467 -4.466 0.001

CaCO3 9.755e-006 9.777e-006 -5.011 -5.010 0.001

CaOH+ 6.563e-009 5.939e-009 -8.183 -8.226 -0.043

CaHSO4+ 8.019e-012 7.256e-012 -11.096 -11.139 -0.043

Cl 8.918e-005

Cl- 8.918e-005 8.055e-005 -4.050 -4.094 -0.044

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.264 -43.263 0.001

K 2.482e-005

K+ 2.480e-005 2.240e-005 -4.606 -4.650 -0.044

KSO4- 1.820e-008 1.647e-008 -7.740 -7.783 -0.043

KOH 1.875e-012 1.879e-012 -11.727 -11.726 0.001

Li 4.758e-006

Li+ 4.756e-006 4.324e-006 -5.323 -5.364 -0.041

LiSO4- 2.714e-009 2.456e-009 -8.566 -8.610 -0.043

LiOH 2.391e-012 2.396e-012 -11.622 -11.621 0.001

Mg 8.972e-004

Mg+2 8.428e-004 5.755e-004 -3.074 -3.240 -0.166

MgHCO3+ 3.954e-005 3.578e-005 -4.403 -4.446 -0.043

MgSO4 1.269e-005 1.272e-005 -4.896 -4.895 0.001

MgCO3 2.151e-006 2.156e-006 -5.667 -5.666 0.001

MgOH+ 1.806e-008 1.634e-008 -7.743 -7.787 -0.043

N(5) 6.000e-006

NO3- 6.000e-006 5.410e-006 -5.222 -5.267 -0.045

Na 2.224e-004

Na+ 2.216e-004 2.007e-004 -3.654 -3.697 -0.043

NaHCO3 6.215e-007 6.229e-007 -6.207 -6.206 0.001

NaSO4- 1.337e-007 1.209e-007 -6.874 -6.917 -0.043

NaCO3- 1.038e-008 9.393e-009 -7.984 -8.027 -0.043

NaOH 3.201e-011 3.208e-011 -10.495 -10.494 0.001

O(0) 2.579e-010

O2 1.289e-010 1.292e-010 -9.890 -9.889 0.001

S(6) 2.398e-004

SO4-2 1.926e-004 1.301e-004 -3.715 -3.886 -0.170

CaSO4 3.410e-005 3.418e-005 -4.467 -4.466 0.001

MgSO4 1.269e-005 1.272e-005 -4.896 -4.895 0.001

SrSO4 1.747e-007 1.751e-007 -6.758 -6.757 0.001

NaSO4- 1.337e-007 1.209e-007 -6.874 -6.917 -0.043

BaSO4 2.630e-008 2.636e-008 -7.580 -7.579 0.001

KSO4- 1.820e-008 1.647e-008 -7.740 -7.783 -0.043

LiSO4- 2.714e-009 2.456e-009 -8.566 -8.610 -0.043

HSO4- 4.509e-010 4.079e-010 -9.346 -9.389 -0.043

CaHSO4+ 8.019e-012 7.256e-012 -11.096 -11.139 -0.043

Si 9.425e-005

H4SiO4 9.401e-005 9.423e-005 -4.027 -4.026 0.001

H3SiO4- 2.364e-007 2.139e-007 -6.626 -6.670 -0.043

H2SiO4-2 2.268e-013 1.520e-013 -12.644 -12.818 -0.174

Sr 1.245e-005

Sr+2 1.176e-005 7.997e-006 -4.930 -5.097 -0.168

SrHCO3+ 4.931e-007 4.476e-007 -6.307 -6.349 -0.042

SrSO4 1.747e-007 1.751e-007 -6.758 -6.757 0.001

SrCO3 1.687e-008 1.691e-008 -7.773 -7.772 0.001

SrOH+ 1.094e-011 9.921e-012 -10.961 -11.003 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.38 -6.72 -4.33 CaSO4

Aragonite 0.11 -8.16 -8.27 CaCO3

Barite -0.10 -10.28 -10.18 BaSO4

Calcite 0.27 -8.16 -8.42 CaCO3

Celestite -2.36 -8.98 -6.62 SrSO4

Chalcedony -0.33 -4.03 -3.70 SiO2

Chrysotile -7.22 26.53 33.75 Mg3Si2O5(OH)4

CO2(g) -1.89 -3.21 -1.31 CO2

Dolomite 0.08 -16.72 -16.80 CaMg(CO3)2

Gypsum -2.13 -6.72 -4.59 CaSO4:2H2O

H2(g) -40.17 -43.26 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.35 -7.79 1.55 NaCl

O2(g) -7.09 -9.89 -2.79 O2

Quartz 0.14 -4.03 -4.16 SiO2

Sepiolite -5.11 10.98 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -7.68 10.98 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.21 -4.03 -2.81 SiO2

Strontianite -1.14 -10.42 -9.28 SrCO3

Talc -4.34 18.48 22.82 Mg3Si4O10(OH)2

Witherite -3.11 -11.72 -8.61 BaCO3

Initial solution 21. 08-8-7

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 6.247e-003 6.247e-003

B 3.425e-006 3.425e-006

Ba 5.901e-007 5.901e-007

Ca 2.249e-003 2.249e-003

Cl 8.551e-005 8.551e-005

K 2.584e-005 2.584e-005

Li 4.902e-006 4.902e-006

Mg 9.383e-004 9.383e-004

N(5) 2.714e-006 2.714e-006

Na 2.215e-004 2.215e-004

S(6) 2.860e-004 2.860e-004

Si 9.958e-005 9.958e-005

Sr 1.405e-005 1.405e-005

----------------------------Description of solution----------------------------

pH = 7.179 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 448

Density (g/cm3) = 0.99982

Activity of water = 1.000

Ionic strength = 9.769e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.233e-003

Total CO2 (mol/kg) = 7.233e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -2.509e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.92

Iterations = 9

Total H = 1.110191e+002

Total O = 5.552848e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

H+ 7.236e-008 6.626e-008 -7.140 -7.179 -0.038

OH- 6.355e-008 5.738e-008 -7.197 -7.241 -0.044

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 3.425e-006

H3BO3 3.399e-006 3.406e-006 -5.469 -5.468 0.001

H2BO3- 2.603e-008 2.355e-008 -7.585 -7.628 -0.043

Ba 5.901e-007

Ba+2 5.461e-007 3.691e-007 -6.263 -6.433 -0.170

BaSO4 2.870e-008 2.876e-008 -7.542 -7.541 0.001

BaHCO3+ 1.483e-008 1.341e-008 -7.829 -7.872 -0.043

BaCO3 4.414e-010 4.424e-010 -9.355 -9.354 0.001

BaOH+ 2.086e-013 1.887e-013 -12.681 -12.724 -0.043

C(4) 7.233e-003

HCO3- 6.093e-003 5.531e-003 -2.215 -2.257 -0.042

CO2 9.972e-004 9.995e-004 -3.001 -3.000 0.001

CaHCO3+ 8.799e-005 7.987e-005 -4.056 -4.098 -0.042

MgHCO3+ 4.136e-005 3.742e-005 -4.383 -4.427 -0.043

CaCO3 5.918e-006 5.932e-006 -5.228 -5.227 0.001

CO3-2 4.349e-006 2.952e-006 -5.362 -5.530 -0.168

MgCO3 1.404e-006 1.407e-006 -5.853 -5.852 0.001

NaHCO3 6.204e-007 6.218e-007 -6.207 -6.206 0.001

SrHCO3+ 5.563e-007 5.049e-007 -6.255 -6.297 -0.042

BaHCO3+ 1.483e-008 1.341e-008 -7.829 -7.872 -0.043

SrCO3 1.187e-008 1.190e-008 -7.925 -7.924 0.001

NaCO3- 6.466e-009 5.850e-009 -8.189 -8.233 -0.043

BaCO3 4.414e-010 4.424e-010 -9.355 -9.354 0.001

Ca 2.249e-003

Ca+2 2.116e-003 1.435e-003 -2.675 -2.843 -0.168

CaHCO3+ 8.799e-005 7.987e-005 -4.056 -4.098 -0.042

CaSO4 3.953e-005 3.962e-005 -4.403 -4.402 0.001

CaCO3 5.918e-006 5.932e-006 -5.228 -5.227 0.001

CaOH+ 3.973e-009 3.595e-009 -8.401 -8.444 -0.043

CaHSO4+ 1.490e-011 1.348e-011 -10.827 -10.870 -0.043

Cl 8.551e-005

Cl- 8.551e-005 7.723e-005 -4.068 -4.112 -0.044

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -42.854 -42.853 0.001

K 2.584e-005

K+ 2.582e-005 2.332e-005 -4.588 -4.632 -0.044

KSO4- 2.264e-008 2.048e-008 -7.645 -7.689 -0.043

KOH 1.217e-012 1.220e-012 -11.915 -11.914 0.001

Li 4.902e-006

Li+ 4.899e-006 4.454e-006 -5.310 -5.351 -0.041

LiSO4- 3.341e-009 3.022e-009 -8.476 -8.520 -0.043

LiOH 1.536e-012 1.540e-012 -11.814 -11.813 0.001

Mg 9.383e-004

Mg+2 8.797e-004 6.005e-004 -3.056 -3.221 -0.166

MgHCO3+ 4.136e-005 3.742e-005 -4.383 -4.427 -0.043

MgSO4 1.582e-005 1.586e-005 -4.801 -4.800 0.001

MgCO3 1.404e-006 1.407e-006 -5.853 -5.852 0.001

MgOH+ 1.176e-008 1.064e-008 -7.930 -7.973 -0.043

N(5) 2.714e-006

NO3- 2.714e-006 2.447e-006 -5.566 -5.611 -0.045

Na 2.215e-004

Na+ 2.207e-004 1.999e-004 -3.656 -3.699 -0.043

NaHCO3 6.204e-007 6.218e-007 -6.207 -6.206 0.001

NaSO4- 1.590e-007 1.439e-007 -6.798 -6.842 -0.043

NaCO3- 6.466e-009 5.850e-009 -8.189 -8.233 -0.043

NaOH 1.989e-011 1.993e-011 -10.701 -10.700 0.001

O(0) 3.905e-011

O2 1.953e-011 1.957e-011 -10.709 -10.708 0.001

S(6) 2.860e-004

SO4-2 2.302e-004 1.555e-004 -3.638 -3.808 -0.171

CaSO4 3.953e-005 3.962e-005 -4.403 -4.402 0.001

MgSO4 1.582e-005 1.586e-005 -4.801 -4.800 0.001

SrSO4 2.349e-007 2.355e-007 -6.629 -6.628 0.001

NaSO4- 1.590e-007 1.439e-007 -6.798 -6.842 -0.043

BaSO4 2.870e-008 2.876e-008 -7.542 -7.541 0.001

KSO4- 2.264e-008 2.048e-008 -7.645 -7.689 -0.043

LiSO4- 3.341e-009 3.022e-009 -8.476 -8.520 -0.043

HSO4- 8.635e-010 7.813e-010 -9.064 -9.107 -0.043

CaHSO4+ 1.490e-011 1.348e-011 -10.827 -10.870 -0.043

Si 9.958e-005

H4SiO4 9.942e-005 9.965e-005 -4.003 -4.002 0.001

H3SiO4- 1.560e-007 1.411e-007 -6.807 -6.850 -0.043

H2SiO4-2 9.338e-014 6.256e-014 -13.030 -13.204 -0.174

Sr 1.405e-005

Sr+2 1.324e-005 9.000e-006 -4.878 -5.046 -0.168

SrHCO3+ 5.563e-007 5.049e-007 -6.255 -6.297 -0.042

SrSO4 2.349e-007 2.355e-007 -6.629 -6.628 0.001

SrCO3 1.187e-008 1.190e-008 -7.925 -7.924 0.001

SrOH+ 7.682e-012 6.965e-012 -11.115 -11.157 -0.043

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.32 -6.65 -4.33 CaSO4

Aragonite -0.10 -8.37 -8.27 CaCO3

Barite -0.06 -10.24 -10.18 BaSO4

Calcite 0.05 -8.37 -8.42 CaCO3

Celestite -2.23 -8.85 -6.62 SrSO4

Chalcedony -0.30 -4.00 -3.70 SiO2

Chrysotile -8.34 25.40 33.75 Mg3Si2O5(OH)4

CO2(g) -1.69 -3.00 -1.31 CO2

Dolomite -0.32 -17.12 -16.80 CaMg(CO3)2

Gypsum -2.06 -6.65 -4.59 CaSO4:2H2O

H2(g) -39.76 -42.85 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.37 -7.81 1.55 NaCl

O2(g) -7.91 -10.71 -2.79 O2

Quartz 0.16 -4.00 -4.16 SiO2

Sepiolite -5.82 10.27 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.39 10.27 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.19 -4.00 -2.81 SiO2

Strontianite -1.30 -10.58 -9.28 SrCO3

Talc -5.42 17.40 22.82 Mg3Si4O10(OH)2

Witherite -3.35 -11.96 -8.61 BaCO3

Initial solution 22. 08-9-21

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 3.708e-007 3.708e-007

Alkalinity 6.264e-003 6.264e-003

B 3.054e-006 3.054e-006

Ba 6.629e-007 6.629e-007

Ca 2.204e-003 2.204e-003

Cl 7.112e-005 7.112e-005

K 2.533e-005 2.533e-005

Li 6.777e-006 6.777e-006

Mg 8.190e-004 8.190e-004

N(5) 2.714e-006 2.714e-006

Na 2.067e-004 2.067e-004

S(6) 2.153e-004 2.153e-004

Si 9.975e-005 9.975e-005

Sr 1.188e-005 1.188e-005

----------------------------Description of solution----------------------------

pH = 7.104 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 433

Density (g/cm3) = 0.99981

Activity of water = 1.000

Ionic strength = 9.362e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.443e-003

Total CO2 (mol/kg) = 7.443e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -4.566e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.61

Iterations = 11

Total H = 1.110191e+002

Total O = 5.552863e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

H+ 8.578e-008 7.866e-008 -7.067 -7.104 -0.038

OH- 5.343e-008 4.833e-008 -7.272 -7.316 -0.044

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 3.708e-007

Al(OH)4- 3.338e-007 3.025e-007 -6.477 -6.519 -0.043

Al(OH)2+ 2.189e-008 1.984e-008 -7.660 -7.703 -0.043

Al(OH)3 1.421e-008 1.424e-008 -7.847 -7.846 0.001

AlOH+2 9.100e-010 6.142e-010 -9.041 -9.212 -0.171

Al+3 2.365e-011 1.084e-011 -10.626 -10.965 -0.339

AlSO4+ 3.815e-012 3.458e-012 -11.419 -11.461 -0.043

Al(SO4)2- 1.350e-014 1.224e-014 -13.870 -13.912 -0.043

AlHSO4+2 3.278e-020 2.212e-020 -19.484 -19.655 -0.171

B 3.054e-006

H3BO3 3.035e-006 3.041e-006 -5.518 -5.517 0.001

H2BO3- 1.954e-008 1.771e-008 -7.709 -7.752 -0.043

Ba 6.629e-007

Ba+2 6.204e-007 4.223e-007 -6.207 -6.374 -0.167

BaSO4 2.506e-008 2.511e-008 -7.601 -7.600 0.001

BaHCO3+ 1.703e-008 1.544e-008 -7.769 -7.811 -0.043

BaCO3 4.279e-010 4.289e-010 -9.369 -9.368 0.001

BaOH+ 2.007e-013 1.819e-013 -12.697 -12.740 -0.043

C(4) 7.443e-003

HCO3- 6.117e-003 5.562e-003 -2.213 -2.255 -0.041

CO2 1.191e-003 1.193e-003 -2.924 -2.923 0.001

CaHCO3+ 8.754e-005 7.960e-005 -4.058 -4.099 -0.041

MgHCO3+ 3.662e-005 3.319e-005 -4.436 -4.479 -0.043

CaCO3 4.969e-006 4.980e-006 -5.304 -5.303 0.001

CO3-2 3.659e-006 2.501e-006 -5.437 -5.602 -0.165

MgCO3 1.049e-006 1.051e-006 -5.979 -5.978 0.001

NaHCO3 5.835e-007 5.847e-007 -6.234 -6.233 0.001

SrHCO3+ 4.772e-007 4.339e-007 -6.321 -6.363 -0.041

BaHCO3+ 1.703e-008 1.544e-008 -7.769 -7.811 -0.043

SrCO3 8.596e-009 8.614e-009 -8.066 -8.065 0.001

NaCO3- 5.112e-009 4.634e-009 -8.291 -8.334 -0.043

BaCO3 4.279e-010 4.289e-010 -9.369 -9.368 0.001

Ca 2.204e-003

Ca+2 2.082e-003 1.422e-003 -2.682 -2.847 -0.165

CaHCO3+ 8.754e-005 7.960e-005 -4.058 -4.099 -0.041

CaSO4 2.989e-005 2.996e-005 -4.524 -4.524 0.001

CaCO3 4.969e-006 4.980e-006 -5.304 -5.303 0.001

CaOH+ 3.310e-009 3.000e-009 -8.480 -8.523 -0.043

CaHSO4+ 1.335e-011 1.210e-011 -10.874 -10.917 -0.043

Cl 7.112e-005

Cl- 7.112e-005 6.435e-005 -4.148 -4.191 -0.043

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -42.705 -42.704 0.001

K 2.533e-005

K+ 2.531e-005 2.291e-005 -4.597 -4.640 -0.043

KSO4- 1.694e-008 1.535e-008 -7.771 -7.814 -0.043

KOH 1.007e-012 1.010e-012 -11.997 -11.996 0.001

Li 6.777e-006

Li+ 6.773e-006 6.168e-006 -5.169 -5.210 -0.041

LiSO4- 3.524e-009 3.194e-009 -8.453 -8.496 -0.043

LiOH 1.792e-012 1.796e-012 -11.747 -11.746 0.001

Mg 8.190e-004

Mg+2 7.706e-004 5.296e-004 -3.113 -3.276 -0.163

MgHCO3+ 3.662e-005 3.319e-005 -4.436 -4.479 -0.043

MgSO4 1.065e-005 1.067e-005 -4.973 -4.972 0.001

MgCO3 1.049e-006 1.051e-006 -5.979 -5.978 0.001

MgOH+ 8.719e-009 7.903e-009 -8.060 -8.102 -0.043

N(5) 2.714e-006

NO3- 2.714e-006 2.452e-006 -5.566 -5.610 -0.044

Na 2.067e-004

Na+ 2.060e-004 1.869e-004 -3.686 -3.728 -0.042

NaHCO3 5.835e-007 5.847e-007 -6.234 -6.233 0.001

NaSO4- 1.133e-007 1.027e-007 -6.946 -6.989 -0.043

NaCO3- 5.112e-009 4.634e-009 -8.291 -8.334 -0.043

NaOH 1.567e-011 1.570e-011 -10.805 -10.804 0.001

O(0) 1.967e-011

O2 9.834e-012 9.855e-012 -11.007 -11.006 0.001

S(6) 2.153e-004

SO4-2 1.744e-004 1.186e-004 -3.758 -3.926 -0.167

CaSO4 2.989e-005 2.996e-005 -4.524 -4.524 0.001

MgSO4 1.065e-005 1.067e-005 -4.973 -4.972 0.001

SrSO4 1.532e-007 1.535e-007 -6.815 -6.814 0.001

NaSO4- 1.133e-007 1.027e-007 -6.946 -6.989 -0.043

BaSO4 2.506e-008 2.511e-008 -7.601 -7.600 0.001

KSO4- 1.694e-008 1.535e-008 -7.771 -7.814 -0.043

LiSO4- 3.524e-009 3.194e-009 -8.453 -8.496 -0.043

HSO4- 7.809e-010 7.078e-010 -9.107 -9.150 -0.043

CaHSO4+ 1.335e-011 1.210e-011 -10.874 -10.917 -0.043

AlSO4+ 3.815e-012 3.458e-012 -11.419 -11.461 -0.043

Al(SO4)2- 1.350e-014 1.224e-014 -13.870 -13.912 -0.043

AlHSO4+2 3.278e-020 2.212e-020 -19.484 -19.655 -0.171

Si 9.975e-005

H4SiO4 9.961e-005 9.983e-005 -4.002 -4.001 0.001

H3SiO4- 1.314e-007 1.191e-007 -6.881 -6.924 -0.043

H2SiO4-2 6.590e-014 4.448e-014 -13.181 -13.352 -0.171

Sr 1.188e-005

Sr+2 1.124e-005 7.690e-006 -4.949 -5.114 -0.165

SrHCO3+ 4.772e-007 4.339e-007 -6.321 -6.363 -0.041

SrSO4 1.532e-007 1.535e-007 -6.815 -6.814 0.001

SrCO3 8.596e-009 8.614e-009 -8.066 -8.065 0.001

SrOH+ 5.519e-012 5.013e-012 -11.258 -11.300 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -1.27 10.35 11.61 Al(OH)3

Albite -3.45 -22.25 -18.80 NaAlSi3O8

Alunite -2.91 -2.76 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.44 -6.77 -4.33 CaSO4

Anorthite -3.82 -23.89 -20.07 CaAl2Si2O8

Aragonite -0.18 -8.45 -8.27 CaCO3

Barite -0.12 -10.30 -10.18 BaSO4

Ca-Montmorillonite 2.27 -44.55 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite -0.03 -8.45 -8.42 CaCO3

Celestite -2.42 -9.04 -6.62 SrSO4

Chalcedony -0.30 -4.00 -3.70 SiO2

Chlorite(14A) -9.68 63.36 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -8.95 24.80 33.75 Mg3Si2O5(OH)4

CO2(g) -1.61 -2.92 -1.31 CO2

Dolomite -0.53 -17.33 -16.80 CaMg(CO3)2

Gibbsite 1.54 10.35 8.81 Al(OH)3

Gypsum -2.19 -6.77 -4.59 CaSO4:2H2O

H2(g) -39.61 -42.70 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.47 -7.92 1.55 NaCl

Illite 0.82 -41.12 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -1.64 -23.16 -21.52 KAlSi3O8

K-mica 6.98 21.51 14.53 KAl3Si3O10(OH)2

Kaolinite 4.17 12.69 8.52 Al2Si2O5(OH)4

O2(g) -8.21 -11.01 -2.79 O2

Quartz 0.16 -4.00 -4.16 SiO2

Sepiolite -6.23 9.86 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.80 9.86 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.19 -4.00 -2.81 SiO2

Strontianite -1.44 -10.72 -9.28 SrCO3

Talc -6.03 16.79 22.82 Mg3Si4O10(OH)2

Witherite -3.37 -11.98 -8.61 BaCO3

Initial solution 23. 08-11-2

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 5.006e-006 5.006e-006

Alkalinity 6.018e-003 6.018e-003

B 2.777e-006 2.777e-006

Ba 6.338e-007 6.338e-007

Ca 2.264e-003 2.264e-003

Cl 6.519e-005 6.519e-005

K 2.687e-005 2.687e-005

Li 4.326e-006 4.326e-006

Mg 9.301e-004 9.301e-004

N(5) 4.929e-006 4.929e-006

Na 2.320e-004 2.320e-004

S(6) 3.026e-004 3.026e-004

Si 1.024e-004 1.024e-004

Sr 1.359e-005 1.359e-005

----------------------------Description of solution----------------------------

pH = 7.168 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 442

Density (g/cm3) = 0.99981

Activity of water = 1.000

Ionic strength = 9.686e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.970e-003

Total CO2 (mol/kg) = 6.970e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = 2.173e-006

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.02

Iterations = 10

Total H = 1.110188e+002

Total O = 5.552781e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

H+ 7.424e-008 6.800e-008 -7.129 -7.168 -0.038

OH- 6.190e-008 5.591e-008 -7.208 -7.253 -0.044

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 5.006e-006

Al(OH)4- 4.603e-006 4.166e-006 -5.337 -5.380 -0.043

Al(OH)2+ 2.256e-007 2.041e-007 -6.647 -6.690 -0.043

Al(OH)3 1.691e-007 1.695e-007 -6.772 -6.771 0.001

AlOH+2 8.143e-009 5.464e-009 -8.089 -8.262 -0.173

Al+3 1.838e-010 8.335e-011 -9.736 -10.079 -0.343

AlSO4+ 4.074e-011 3.688e-011 -10.390 -10.433 -0.043

Al(SO4)2- 2.000e-013 1.810e-013 -12.699 -12.742 -0.043

AlHSO4+2 3.040e-019 2.040e-019 -18.517 -18.690 -0.173

B 2.777e-006

H3BO3 2.756e-006 2.762e-006 -5.560 -5.559 0.001

H2BO3- 2.056e-008 1.861e-008 -7.687 -7.730 -0.043

Ba 6.338e-007

Ba+2 5.855e-007 3.963e-007 -6.232 -6.402 -0.169

BaSO4 3.260e-008 3.268e-008 -7.487 -7.486 0.001

BaHCO3+ 1.528e-008 1.383e-008 -7.816 -7.859 -0.043

BaCO3 4.436e-010 4.446e-010 -9.353 -9.352 0.001

BaOH+ 2.182e-013 1.974e-013 -12.661 -12.705 -0.043

C(4) 6.970e-003

HCO3- 5.850e-003 5.312e-003 -2.233 -2.275 -0.042

CO2 9.830e-004 9.852e-004 -3.007 -3.006 0.001

CaHCO3+ 8.522e-005 7.738e-005 -4.069 -4.111 -0.042

MgHCO3+ 3.945e-005 3.570e-005 -4.404 -4.447 -0.043

CaCO3 5.588e-006 5.600e-006 -5.253 -5.252 0.001

CO3-2 4.065e-006 2.763e-006 -5.391 -5.559 -0.168

MgCO3 1.305e-006 1.308e-006 -5.884 -5.883 0.001

NaHCO3 6.243e-007 6.256e-007 -6.205 -6.204 0.001

SrHCO3+ 5.178e-007 4.701e-007 -6.286 -6.328 -0.042

BaHCO3+ 1.528e-008 1.383e-008 -7.816 -7.859 -0.043

SrCO3 1.077e-008 1.080e-008 -7.968 -7.967 0.001

NaCO3- 6.337e-009 5.735e-009 -8.198 -8.241 -0.043

BaCO3 4.436e-010 4.446e-010 -9.353 -9.352 0.001

Ca 2.264e-003

Ca+2 2.131e-003 1.448e-003 -2.671 -2.839 -0.168

CaHCO3+ 8.522e-005 7.738e-005 -4.069 -4.111 -0.042

CaSO4 4.219e-005 4.229e-005 -4.375 -4.374 0.001

CaCO3 5.588e-006 5.600e-006 -5.253 -5.252 0.001

CaOH+ 3.904e-009 3.533e-009 -8.409 -8.452 -0.043

CaHSO4+ 1.632e-011 1.477e-011 -10.787 -10.831 -0.043

Cl 6.519e-005

Cl- 6.519e-005 5.890e-005 -4.186 -4.230 -0.044

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -42.832 -42.831 0.001

K 2.687e-005

K+ 2.684e-005 2.425e-005 -4.571 -4.615 -0.044

KSO4- 2.490e-008 2.254e-008 -7.604 -7.647 -0.043

KOH 1.234e-012 1.236e-012 -11.909 -11.908 0.001

Li 4.326e-006

Li+ 4.323e-006 3.931e-006 -5.364 -5.405 -0.041

LiSO4- 3.119e-009 2.823e-009 -8.506 -8.549 -0.043

LiOH 1.321e-012 1.324e-012 -11.879 -11.878 0.001

Mg 9.301e-004

Mg+2 8.727e-004 5.965e-004 -3.059 -3.224 -0.165

MgHCO3+ 3.945e-005 3.570e-005 -4.404 -4.447 -0.043

MgSO4 1.663e-005 1.667e-005 -4.779 -4.778 0.001

MgCO3 1.305e-006 1.308e-006 -5.884 -5.883 0.001

MgOH+ 1.138e-008 1.030e-008 -7.944 -7.987 -0.043

N(5) 4.929e-006

NO3- 4.929e-006 4.445e-006 -5.307 -5.352 -0.045

Na 2.320e-004

Na+ 2.312e-004 2.094e-004 -3.636 -3.679 -0.043

NaHCO3 6.243e-007 6.256e-007 -6.205 -6.204 0.001

NaSO4- 1.763e-007 1.595e-007 -6.754 -6.797 -0.043

NaCO3- 6.337e-009 5.735e-009 -8.198 -8.241 -0.043

NaOH 2.030e-011 2.035e-011 -10.692 -10.692 0.001

O(0) 3.521e-011

O2 1.761e-011 1.764e-011 -10.754 -10.753 0.001

S(6) 3.026e-004

SO4-2 2.433e-004 1.645e-004 -3.614 -3.784 -0.170

CaSO4 4.219e-005 4.229e-005 -4.375 -4.374 0.001

MgSO4 1.663e-005 1.667e-005 -4.779 -4.778 0.001

SrSO4 2.410e-007 2.416e-007 -6.618 -6.617 0.001

NaSO4- 1.763e-007 1.595e-007 -6.754 -6.797 -0.043

BaSO4 3.260e-008 3.268e-008 -7.487 -7.486 0.001

KSO4- 2.490e-008 2.254e-008 -7.604 -7.647 -0.043

LiSO4- 3.119e-009 2.823e-009 -8.506 -8.549 -0.043

HSO4- 9.374e-010 8.484e-010 -9.028 -9.071 -0.043

AlSO4+ 4.074e-011 3.688e-011 -10.390 -10.433 -0.043

CaHSO4+ 1.632e-011 1.477e-011 -10.787 -10.831 -0.043

Al(SO4)2- 2.000e-013 1.810e-013 -12.699 -12.742 -0.043

AlHSO4+2 3.040e-019 2.040e-019 -18.517 -18.690 -0.173

Si 1.024e-004

H4SiO4 1.023e-004 1.025e-004 -3.990 -3.989 0.001

H3SiO4- 1.562e-007 1.414e-007 -6.806 -6.850 -0.043

H2SiO4-2 9.105e-014 6.110e-014 -13.041 -13.214 -0.173

Sr 1.359e-005

Sr+2 1.282e-005 8.725e-006 -4.892 -5.059 -0.167

SrHCO3+ 5.178e-007 4.701e-007 -6.286 -6.328 -0.042

SrSO4 2.410e-007 2.416e-007 -6.618 -6.617 0.001

SrCO3 1.077e-008 1.080e-008 -7.968 -7.967 0.001

SrOH+ 7.253e-012 6.579e-012 -11.139 -11.182 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -0.19 11.42 11.61 Al(OH)3

Albite -2.23 -21.03 -18.80 NaAlSi3O8

Alunite 0.44 0.58 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.29 -6.62 -4.33 CaSO4

Anorthite -1.51 -21.58 -20.07 CaAl2Si2O8

Aragonite -0.13 -8.40 -8.27 CaCO3

Barite -0.00 -10.19 -10.18 BaSO4

Ca-Montmorillonite 4.84 -41.98 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.02 -8.40 -8.42 CaCO3

Celestite -2.22 -8.84 -6.62 SrSO4

Chalcedony -0.29 -3.99 -3.70 SiO2

Chlorite(14A) -6.61 66.43 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -8.40 25.35 33.75 Mg3Si2O5(OH)4

CO2(g) -1.69 -3.01 -1.31 CO2

Dolomite -0.38 -17.18 -16.80 CaMg(CO3)2

Gibbsite 2.61 11.42 8.81 Al(OH)3

Gypsum -2.04 -6.62 -4.59 CaSO4:2H2O

H2(g) -39.74 -42.83 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.46 -7.91 1.55 NaCl

Illite 3.44 -38.51 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -0.44 -21.96 -21.52 KAlSi3O8

K-mica 10.33 24.85 14.53 KAl3Si3O10(OH)2

Kaolinite 6.35 14.87 8.52 Al2Si2O5(OH)4

O2(g) -7.96 -10.75 -2.79 O2

Quartz 0.18 -3.99 -4.16 SiO2

Sepiolite -5.84 10.25 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -8.41 10.25 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.17 -3.99 -2.81 SiO2

Strontianite -1.34 -10.62 -9.28 SrCO3

Talc -5.45 17.37 22.82 Mg3Si4O10(OH)2

Witherite -3.35 -11.96 -8.61 BaCO3

Initial solution 24. 08-11-30

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 2.889e-005 2.889e-005

Alkalinity 6.165e-003 6.165e-003

B 3.054e-006 3.054e-006

Ba 6.120e-007 6.120e-007

Ca 2.304e-003 2.304e-003

Cl 1.036e-004 1.036e-004

K 3.045e-005 3.045e-005

Li 6.633e-006 6.633e-006

Mg 9.795e-004 9.795e-004

N(5) 5.572e-006 5.572e-006

Na 2.311e-004 2.311e-004

S(6) 3.177e-004 3.177e-004

Si 1.239e-004 1.239e-004

Sr 1.393e-005 1.393e-005

----------------------------Description of solution----------------------------

pH = 7.236 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 452

Density (g/cm3) = 0.99982

Activity of water = 1.000

Ionic strength = 9.930e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.884e-003

Total CO2 (mol/kg) = 6.884e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = 4.133e-005

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.31

Iterations = 11

Total H = 1.110191e+002

Total O = 5.552793e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 7.260e-008 6.550e-008 -7.139 -7.184 -0.045

H+ 6.342e-008 5.804e-008 -7.198 -7.236 -0.039

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 2.889e-005

Al(OH)4- 2.704e-005 2.445e-005 -4.568 -4.612 -0.044

Al(OH)2+ 9.655e-007 8.729e-007 -6.015 -6.059 -0.044

Al(OH)3 8.472e-007 8.492e-007 -6.072 -6.071 0.001

AlOH+2 2.985e-008 1.994e-008 -7.525 -7.700 -0.175

Al+3 5.768e-010 2.597e-010 -9.239 -9.586 -0.347

AlSO4+ 1.324e-010 1.197e-010 -9.878 -9.922 -0.044

Al(SO4)2- 6.770e-013 6.121e-013 -12.169 -12.213 -0.044

AlHSO4+2 8.457e-019 5.650e-019 -18.073 -18.248 -0.175

B 3.054e-006

H3BO3 3.028e-006 3.035e-006 -5.519 -5.518 0.001

H2BO3- 2.649e-008 2.395e-008 -7.577 -7.621 -0.044

Ba 6.120e-007

Ba+2 5.641e-007 3.802e-007 -6.249 -6.420 -0.171

BaSO4 3.259e-008 3.266e-008 -7.487 -7.486 0.001

BaHCO3+ 1.478e-008 1.336e-008 -7.830 -7.874 -0.044

BaCO3 5.020e-010 5.031e-010 -9.299 -9.298 0.001

BaOH+ 2.455e-013 2.219e-013 -12.610 -12.654 -0.044

C(4) 6.884e-003

HCO3- 5.896e-003 5.349e-003 -2.229 -2.272 -0.042

CO2 8.447e-004 8.466e-004 -3.073 -3.072 0.001

CaHCO3+ 8.694e-005 7.886e-005 -4.061 -4.103 -0.042

MgHCO3+ 4.166e-005 3.767e-005 -4.380 -4.424 -0.044

CaCO3 6.671e-006 6.686e-006 -5.176 -5.175 0.001

CO3-2 4.814e-006 3.259e-006 -5.317 -5.487 -0.169

MgCO3 1.613e-006 1.617e-006 -5.792 -5.791 0.001

NaHCO3 6.254e-007 6.269e-007 -6.204 -6.203 0.001

SrHCO3+ 5.323e-007 4.829e-007 -6.274 -6.316 -0.042

BaHCO3+ 1.478e-008 1.336e-008 -7.830 -7.874 -0.044

SrCO3 1.296e-008 1.299e-008 -7.887 -7.886 0.001

NaCO3- 7.447e-009 6.733e-009 -8.128 -8.172 -0.044

BaCO3 5.020e-010 5.031e-010 -9.299 -9.298 0.001

Ca 2.304e-003

Ca+2 2.166e-003 1.466e-003 -2.664 -2.834 -0.170

CaHCO3+ 8.694e-005 7.886e-005 -4.061 -4.103 -0.042

CaSO4 4.449e-005 4.459e-005 -4.352 -4.351 0.001

CaCO3 6.671e-006 6.686e-006 -5.176 -5.175 0.001

CaOH+ 4.634e-009 4.190e-009 -8.334 -8.378 -0.044

CaHSO4+ 1.470e-011 1.329e-011 -10.833 -10.876 -0.044

Cl 1.036e-004

Cl- 1.036e-004 9.347e-005 -3.985 -4.029 -0.045

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -42.969 -42.968 0.001

K 3.045e-005

K+ 3.042e-005 2.745e-005 -4.517 -4.561 -0.045

KSO4- 2.940e-008 2.658e-008 -7.532 -7.575 -0.044

KOH 1.636e-012 1.640e-012 -11.786 -11.785 0.001

Li 6.633e-006

Li+ 6.628e-006 6.022e-006 -5.179 -5.220 -0.042

LiSO4- 4.983e-009 4.505e-009 -8.302 -8.346 -0.044

LiOH 2.371e-012 2.376e-012 -11.625 -11.624 0.001

Mg 9.795e-004

Mg+2 9.180e-004 6.250e-004 -3.037 -3.204 -0.167

MgHCO3+ 4.166e-005 3.767e-005 -4.380 -4.424 -0.044

MgSO4 1.816e-005 1.820e-005 -4.741 -4.740 0.001

MgCO3 1.613e-006 1.617e-006 -5.792 -5.791 0.001

MgOH+ 1.398e-008 1.264e-008 -7.854 -7.898 -0.044

N(5) 5.572e-006

NO3- 5.572e-006 5.019e-006 -5.254 -5.299 -0.045

Na 2.311e-004

Na+ 2.303e-004 2.084e-004 -3.638 -3.681 -0.043

NaHCO3 6.254e-007 6.269e-007 -6.204 -6.203 0.001

NaSO4- 1.829e-007 1.654e-007 -6.738 -6.781 -0.044

NaCO3- 7.447e-009 6.733e-009 -8.128 -8.172 -0.044

NaOH 2.367e-011 2.372e-011 -10.626 -10.625 0.001

O(0) 6.633e-011

O2 3.317e-011 3.324e-011 -10.479 -10.478 0.001

S(6) 3.177e-004

SO4-2 2.545e-004 1.714e-004 -3.594 -3.766 -0.172

CaSO4 4.449e-005 4.459e-005 -4.352 -4.351 0.001

MgSO4 1.816e-005 1.820e-005 -4.741 -4.740 0.001

SrSO4 2.561e-007 2.567e-007 -6.592 -6.591 0.001

NaSO4- 1.829e-007 1.654e-007 -6.738 -6.781 -0.044

BaSO4 3.259e-008 3.266e-008 -7.487 -7.486 0.001

KSO4- 2.940e-008 2.658e-008 -7.532 -7.575 -0.044

LiSO4- 4.983e-009 4.505e-009 -8.302 -8.346 -0.044

HSO4- 8.346e-010 7.545e-010 -9.079 -9.122 -0.044

AlSO4+ 1.324e-010 1.197e-010 -9.878 -9.922 -0.044

CaHSO4+ 1.470e-011 1.329e-011 -10.833 -10.876 -0.044

Al(SO4)2- 6.770e-013 6.121e-013 -12.169 -12.213 -0.044

AlHSO4+2 8.457e-019 5.650e-019 -18.073 -18.248 -0.175

Si 1.239e-004

H4SiO4 1.237e-004 1.240e-004 -3.908 -3.907 0.001

H3SiO4- 2.216e-007 2.004e-007 -6.654 -6.698 -0.044

H2SiO4-2 1.518e-013 1.014e-013 -12.819 -12.994 -0.175

Sr 1.393e-005

Sr+2 1.313e-005 8.900e-006 -4.882 -5.051 -0.169

SrHCO3+ 5.323e-007 4.829e-007 -6.274 -6.316 -0.042

SrSO4 2.561e-007 2.567e-007 -6.592 -6.591 0.001

SrCO3 1.296e-008 1.299e-008 -7.887 -7.886 0.001

SrOH+ 8.678e-012 7.863e-012 -11.062 -11.104 -0.043

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) 0.51 12.12 11.61 Al(OH)3

Albite -1.21 -20.01 -18.80 NaAlSi3O8

Alunite 2.42 2.57 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.27 -6.60 -4.33 CaSO4

Anorthite 0.20 -19.87 -20.07 CaAl2Si2O8

Aragonite -0.05 -8.32 -8.27 CaCO3

Barite -0.00 -10.19 -10.18 BaSO4

Ca-Montmorillonite 6.80 -40.02 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.10 -8.32 -8.42 CaCO3

Celestite -2.19 -8.82 -6.62 SrSO4

Chalcedony -0.21 -3.91 -3.70 SiO2

Chlorite(14A) -4.17 68.87 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -7.76 25.99 33.75 Mg3Si2O5(OH)4

CO2(g) -1.76 -3.07 -1.31 CO2

Dolomite -0.21 -17.01 -16.80 CaMg(CO3)2

Gibbsite 3.31 12.12 8.81 Al(OH)3

Gypsum -2.01 -6.60 -4.59 CaSO4:2H2O

H2(g) -39.87 -42.97 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.26 -7.71 1.55 NaCl

Illite 5.45 -36.50 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar 0.63 -20.89 -21.52 KAlSi3O8

K-mica 12.80 27.32 14.53 KAl3Si3O10(OH)2

Kaolinite 7.91 16.43 8.52 Al2Si2O5(OH)4

O2(g) -7.68 -10.48 -2.79 O2

Quartz 0.26 -3.91 -4.16 SiO2

Sepiolite -5.27 10.82 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -7.84 10.82 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.09 -3.91 -2.81 SiO2

Strontianite -1.26 -10.54 -9.28 SrCO3

Talc -4.65 18.18 22.82 Mg3Si4O10(OH)2

Witherite -3.30 -11.91 -8.61 BaCO3

Initial solution 25. 09-1-6

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 1.372e-006 1.372e-006

Alkalinity 5.936e-003 5.936e-003

B 1.851e-006 1.851e-006

Ba 6.119e-007 6.119e-007

Ca 2.144e-003 2.144e-003

Cl 6.293e-005 6.293e-005

K 9.723e-006 9.723e-006

Li 1.586e-006 1.586e-006

Mg 7.860e-004 7.860e-004

N(5) 1.786e-006 1.786e-006

Na 1.911e-004 1.911e-004

S(6) 2.996e-004 2.996e-004

Si 8.126e-005 8.126e-005

Sr 1.073e-005 1.073e-005

----------------------------Description of solution----------------------------

pH = 7.429 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 420

Density (g/cm3) = 0.99980

Activity of water = 1.000

Ionic strength = 9.104e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.444e-003

Total CO2 (mol/kg) = 6.444e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -5.098e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -4.18

Iterations = 10

Total H = 1.110187e+002

Total O = 5.552656e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.127e-007 1.021e-007 -6.948 -6.991 -0.043

H+ 4.056e-008 3.723e-008 -7.392 -7.429 -0.037

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 1.372e-006

Al(OH)4- 1.325e-006 1.203e-006 -5.878 -5.920 -0.042

Al(OH)3 2.674e-008 2.679e-008 -7.573 -7.572 0.001

Al(OH)2+ 1.947e-008 1.767e-008 -7.711 -7.753 -0.042

AlOH+2 3.817e-010 2.589e-010 -9.418 -9.587 -0.169

Al+3 4.677e-012 2.162e-012 -11.330 -11.665 -0.335

AlSO4+ 1.068e-012 9.695e-013 -11.971 -12.013 -0.042

Al(SO4)2- 5.317e-015 4.825e-015 -14.274 -14.317 -0.042

AlHSO4+2 4.329e-021 2.936e-021 -20.364 -20.532 -0.169

B 1.851e-006

H3BO3 1.826e-006 1.830e-006 -5.738 -5.738 0.001

H2BO3- 2.481e-008 2.252e-008 -7.605 -7.647 -0.042

Ba 6.119e-007

Ba+2 5.643e-007 3.859e-007 -6.249 -6.414 -0.165

BaSO4 3.219e-008 3.226e-008 -7.492 -7.491 0.001

BaHCO3+ 1.469e-008 1.333e-008 -7.833 -7.875 -0.042

BaCO3 7.812e-010 7.828e-010 -9.107 -9.106 0.001

BaOH+ 3.870e-013 3.512e-013 -12.412 -12.454 -0.042

C(4) 6.444e-003

HCO3- 5.777e-003 5.259e-003 -2.238 -2.279 -0.041

CO2 5.329e-004 5.340e-004 -3.273 -3.272 0.001

CaHCO3+ 8.032e-005 7.312e-005 -4.095 -4.136 -0.041

MgHCO3+ 3.319e-005 3.012e-005 -4.479 -4.521 -0.042

CaCO3 9.644e-006 9.665e-006 -5.016 -5.015 0.001

CO3-2 7.276e-006 4.997e-006 -5.138 -5.301 -0.163

MgCO3 2.011e-006 2.016e-006 -5.696 -5.696 0.001

NaHCO3 5.104e-007 5.115e-007 -6.292 -6.291 0.001

SrHCO3+ 4.075e-007 3.710e-007 -6.390 -6.431 -0.041

SrCO3 1.553e-008 1.556e-008 -7.809 -7.808 0.001

BaHCO3+ 1.469e-008 1.333e-008 -7.833 -7.875 -0.042

NaCO3- 9.438e-009 8.565e-009 -8.025 -8.067 -0.042

BaCO3 7.812e-010 7.828e-010 -9.107 -9.106 0.001

Ca 2.144e-003

Ca+2 2.014e-003 1.382e-003 -2.696 -2.860 -0.164

CaHCO3+ 8.032e-005 7.312e-005 -4.095 -4.136 -0.041

CaSO4 4.083e-005 4.091e-005 -4.389 -4.388 0.001

CaCO3 9.644e-006 9.665e-006 -5.016 -5.015 0.001

CaOH+ 6.787e-009 6.159e-009 -8.168 -8.210 -0.042

CaHSO4+ 8.620e-012 7.823e-012 -11.064 -11.107 -0.042

Cl 6.293e-005

Cl- 6.293e-005 5.702e-005 -4.201 -4.244 -0.043

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.355 -43.354 0.001

K 9.723e-006

K+ 9.714e-006 8.801e-006 -5.013 -5.055 -0.043

KSO4- 9.137e-009 8.292e-009 -8.039 -8.081 -0.042

KOH 8.179e-013 8.196e-013 -12.087 -12.086 0.001

Li 1.586e-006

Li+ 1.585e-006 1.445e-006 -5.800 -5.840 -0.040

LiSO4- 1.159e-009 1.052e-009 -8.936 -8.978 -0.042

LiOH 8.871e-013 8.890e-013 -12.052 -12.051 0.001

Mg 7.860e-004

Mg+2 7.364e-004 5.083e-004 -3.133 -3.294 -0.161

MgHCO3+ 3.319e-005 3.012e-005 -4.479 -4.521 -0.042

MgSO4 1.437e-005 1.440e-005 -4.843 -4.842 0.001

MgCO3 2.011e-006 2.016e-006 -5.696 -5.696 0.001

MgOH+ 1.766e-008 1.603e-008 -7.753 -7.795 -0.042

N(5) 1.786e-006

NO3- 1.786e-006 1.615e-006 -5.748 -5.792 -0.044

Na 1.911e-004

Na+ 1.904e-004 1.729e-004 -3.720 -3.762 -0.042

NaHCO3 5.104e-007 5.115e-007 -6.292 -6.291 0.001

NaSO4- 1.472e-007 1.335e-007 -6.832 -6.874 -0.042

NaCO3- 9.438e-009 8.565e-009 -8.025 -8.067 -0.042

NaOH 3.062e-011 3.069e-011 -10.514 -10.513 0.001

O(0) 3.920e-010

O2 1.960e-010 1.964e-010 -9.708 -9.707 0.001

S(6) 2.996e-004

SO4-2 2.441e-004 1.668e-004 -3.613 -3.778 -0.165

CaSO4 4.083e-005 4.091e-005 -4.389 -4.388 0.001

MgSO4 1.437e-005 1.440e-005 -4.843 -4.842 0.001

SrSO4 1.948e-007 1.952e-007 -6.710 -6.710 0.001

NaSO4- 1.472e-007 1.335e-007 -6.832 -6.874 -0.042

BaSO4 3.219e-008 3.226e-008 -7.492 -7.491 0.001

KSO4- 9.137e-009 8.292e-009 -8.039 -8.081 -0.042

LiSO4- 1.159e-009 1.052e-009 -8.936 -8.978 -0.042

HSO4- 5.189e-010 4.709e-010 -9.285 -9.327 -0.042

CaHSO4+ 8.620e-012 7.823e-012 -11.064 -11.107 -0.042

AlSO4+ 1.068e-012 9.695e-013 -11.971 -12.013 -0.042

Al(SO4)2- 5.317e-015 4.825e-015 -14.274 -14.317 -0.042

AlHSO4+2 4.329e-021 2.936e-021 -20.364 -20.532 -0.169

Si 8.126e-005

H4SiO4 8.104e-005 8.121e-005 -4.091 -4.090 0.001

H3SiO4- 2.255e-007 2.047e-007 -6.647 -6.689 -0.042

H2SiO4-2 2.381e-013 1.615e-013 -12.623 -12.792 -0.169

Sr 1.073e-005

Sr+2 1.012e-005 6.954e-006 -4.995 -5.158 -0.163

SrHCO3+ 4.075e-007 3.710e-007 -6.390 -6.431 -0.041

SrSO4 1.948e-007 1.952e-007 -6.710 -6.710 0.001

SrCO3 1.553e-008 1.556e-008 -7.809 -7.808 0.001

SrOH+ 1.053e-011 9.579e-012 -10.977 -11.019 -0.041

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -0.99 10.62 11.61 Al(OH)3

Albite -3.15 -21.95 -18.80 NaAlSi3O8

Alunite -3.18 -3.03 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.30 -6.64 -4.33 CaSO4

Anorthite -2.81 -22.88 -20.07 CaAl2Si2O8

Aragonite 0.11 -8.16 -8.27 CaCO3

Barite -0.01 -10.19 -10.18 BaSO4

Ca-Montmorillonite 2.69 -44.13 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.26 -8.16 -8.42 CaCO3

Celestite -2.31 -8.94 -6.62 SrSO4

Chalcedony -0.39 -4.09 -3.70 SiO2

Chlorite(14A) -6.24 66.79 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -7.24 26.51 33.75 Mg3Si2O5(OH)4

CO2(g) -1.96 -3.27 -1.31 CO2

Dolomite 0.04 -16.76 -16.80 CaMg(CO3)2

Gibbsite 1.81 10.62 8.81 Al(OH)3

Gypsum -2.05 -6.64 -4.59 CaSO4:2H2O

H2(g) -40.26 -43.35 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.56 -8.01 1.55 NaCl

Illite 1.25 -40.70 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -1.73 -23.25 -21.52 KAlSi3O8

K-mica 7.44 21.97 14.53 KAl3Si3O10(OH)2

Kaolinite 4.54 13.06 8.52 Al2Si2O5(OH)4

O2(g) -6.91 -9.71 -2.79 O2

Quartz 0.07 -4.09 -4.16 SiO2

Sepiolite -5.23 10.86 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -7.80 10.86 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.28 -4.09 -2.81 SiO2

Strontianite -1.18 -10.46 -9.28 SrCO3

Talc -4.49 18.33 22.82 Mg3Si4O10(OH)2

Witherite -3.10 -11.71 -8.61 BaCO3

Initial solution 26. 09-2-21

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 1.431e-005 1.431e-005

Alkalinity 5.755e-003 5.755e-003

B 1.759e-006 1.759e-006

Ba 6.338e-007 6.338e-007

Ca 2.309e-003 2.309e-003

Cl 6.209e-005 6.209e-005

K 1.203e-005 1.203e-005

Li 5.335e-006 5.335e-006

Mg 8.189e-004 8.189e-004

N(5) 1.929e-006 1.929e-006

Na 1.902e-004 1.902e-004

S(6) 3.535e-004 3.535e-004

Si 9.208e-005 9.208e-005

Sr 1.005e-005 1.005e-005

----------------------------Description of solution----------------------------

pH = 7.873 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 428

Density (g/cm3) = 0.99980

Activity of water = 1.000

Ionic strength = 9.398e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 5.827e-003

Total CO2 (mol/kg) = 5.827e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = 1.638e-006

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.01

Iterations = 11

Total H = 1.110185e+002

Total O = 5.552537e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 3.140e-007 2.840e-007 -6.503 -6.547 -0.044

H+ 1.460e-008 1.339e-008 -7.836 -7.873 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 1.431e-005

Al(OH)4- 1.418e-005 1.285e-005 -4.848 -4.891 -0.043

Al(OH)3 1.027e-007 1.030e-007 -6.988 -6.987 0.001

Al(OH)2+ 2.694e-008 2.441e-008 -7.570 -7.612 -0.043

AlOH+2 1.907e-010 1.286e-010 -9.720 -9.891 -0.171

Al+3 8.437e-013 3.863e-013 -12.074 -12.413 -0.339

AlSO4+ 2.223e-013 2.015e-013 -12.653 -12.696 -0.043

Al(SO4)2- 1.287e-015 1.166e-015 -14.891 -14.933 -0.043

AlHSO4+2 3.252e-022 2.194e-022 -21.488 -21.659 -0.171

B 1.759e-006

H3BO3 1.694e-006 1.698e-006 -5.771 -5.770 0.001

H2BO3- 6.411e-008 5.810e-008 -7.193 -7.236 -0.043

Ba 6.338e-007

Ba+2 5.792e-007 3.941e-007 -6.237 -6.404 -0.167

BaSO4 3.822e-008 3.831e-008 -7.418 -7.417 0.001

BaHCO3+ 1.423e-008 1.290e-008 -7.847 -7.890 -0.043

BaCO3 2.101e-009 2.106e-009 -8.678 -8.677 0.001

BaOH+ 1.100e-012 9.973e-013 -11.958 -12.001 -0.043

C(4) 5.827e-003

HCO3- 5.479e-003 4.981e-003 -2.261 -2.303 -0.041

CO2 1.815e-004 1.819e-004 -3.741 -3.740 0.001

CaHCO3+ 8.094e-005 7.359e-005 -4.092 -4.133 -0.041

MgHCO3+ 3.249e-005 2.944e-005 -4.488 -4.531 -0.043

CaCO3 2.699e-005 2.705e-005 -4.569 -4.568 0.001

CO3-2 1.926e-005 1.316e-005 -4.715 -4.881 -0.165

MgCO3 5.467e-006 5.479e-006 -5.262 -5.261 0.001

NaHCO3 4.805e-007 4.816e-007 -6.318 -6.317 0.001

SrHCO3+ 3.589e-007 3.263e-007 -6.445 -6.486 -0.041

SrCO3 3.798e-008 3.806e-008 -7.420 -7.419 0.001

NaCO3- 2.474e-008 2.243e-008 -7.607 -7.649 -0.043

BaHCO3+ 1.423e-008 1.290e-008 -7.847 -7.890 -0.043

BaCO3 2.101e-009 2.106e-009 -8.678 -8.677 0.001

Ca 2.309e-003

Ca+2 2.151e-003 1.468e-003 -2.667 -2.833 -0.166

CaHCO3+ 8.094e-005 7.359e-005 -4.092 -4.133 -0.041

CaSO4 5.045e-005 5.056e-005 -4.297 -4.296 0.001

CaCO3 2.699e-005 2.705e-005 -4.569 -4.568 0.001

CaOH+ 2.008e-008 1.820e-008 -7.697 -7.740 -0.043

CaHSO4+ 3.836e-012 3.477e-012 -11.416 -11.459 -0.043

Cl 6.209e-005

Cl- 6.209e-005 5.617e-005 -4.207 -4.250 -0.043

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -44.244 -44.243 0.001

K 1.203e-005

K+ 1.201e-005 1.087e-005 -4.920 -4.964 -0.043

KSO4- 1.314e-008 1.191e-008 -7.881 -7.924 -0.043

KOH 2.809e-012 2.815e-012 -11.552 -11.551 0.001

Li 5.335e-006

Li+ 5.330e-006 4.853e-006 -5.273 -5.314 -0.041

LiSO4- 4.534e-009 4.109e-009 -8.343 -8.386 -0.043

LiOH 8.286e-012 8.304e-012 -11.082 -11.081 0.001

Mg 8.189e-004

Mg+2 7.637e-004 5.245e-004 -3.117 -3.280 -0.163

MgHCO3+ 3.249e-005 2.944e-005 -4.488 -4.531 -0.043

MgSO4 1.725e-005 1.728e-005 -4.763 -4.762 0.001

MgCO3 5.467e-006 5.479e-006 -5.262 -5.261 0.001

MgOH+ 5.075e-008 4.599e-008 -7.295 -7.337 -0.043

N(5) 1.929e-006

NO3- 1.929e-006 1.742e-006 -5.715 -5.759 -0.044

Na 1.902e-004

Na+ 1.895e-004 1.719e-004 -3.722 -3.765 -0.042

NaHCO3 4.805e-007 4.816e-007 -6.318 -6.317 0.001

NaSO4- 1.704e-007 1.544e-007 -6.769 -6.811 -0.043

NaCO3- 2.474e-008 2.243e-008 -7.607 -7.649 -0.043

NaOH 8.466e-011 8.484e-011 -10.072 -10.071 0.001

O(0) 2.344e-008

O2 1.172e-008 1.175e-008 -7.931 -7.930 0.001

S(6) 3.535e-004

SO4-2 2.854e-004 1.940e-004 -3.545 -3.712 -0.168

CaSO4 5.045e-005 5.056e-005 -4.297 -4.296 0.001

MgSO4 1.725e-005 1.728e-005 -4.763 -4.762 0.001

SrSO4 2.103e-007 2.108e-007 -6.677 -6.676 0.001

NaSO4- 1.704e-007 1.544e-007 -6.769 -6.811 -0.043

BaSO4 3.822e-008 3.831e-008 -7.418 -7.417 0.001

KSO4- 1.314e-008 1.191e-008 -7.881 -7.924 -0.043

LiSO4- 4.534e-009 4.109e-009 -8.343 -8.386 -0.043

HSO4- 2.173e-010 1.969e-010 -9.663 -9.706 -0.043

CaHSO4+ 3.836e-012 3.477e-012 -11.416 -11.459 -0.043

AlSO4+ 2.223e-013 2.015e-013 -12.653 -12.696 -0.043

Al(SO4)2- 1.287e-015 1.166e-015 -14.891 -14.933 -0.043

AlHSO4+2 3.252e-022 2.194e-022 -21.488 -21.659 -0.171

Si 9.208e-005

H4SiO4 9.138e-005 9.157e-005 -4.039 -4.038 0.001

H3SiO4- 7.082e-007 6.418e-007 -6.150 -6.193 -0.043

H2SiO4-2 2.088e-012 1.409e-012 -11.680 -11.851 -0.171

Sr 1.005e-005

Sr+2 9.441e-006 6.457e-006 -5.025 -5.190 -0.165

SrHCO3+ 3.589e-007 3.263e-007 -6.445 -6.486 -0.041

SrSO4 2.103e-007 2.108e-007 -6.677 -6.676 0.001

SrCO3 3.798e-008 3.806e-008 -7.420 -7.419 0.001

SrOH+ 2.724e-011 2.474e-011 -10.565 -10.607 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -0.41 11.21 11.61 Al(OH)3

Albite -1.97 -20.77 -18.80 NaAlSi3O8

Alunite -2.53 -2.39 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.21 -6.55 -4.33 CaSO4

Anorthite -0.62 -20.69 -20.07 CaAl2Si2O8

Aragonite 0.56 -7.71 -8.27 CaCO3

Barite 0.07 -10.12 -10.18 BaSO4

Ca-Montmorillonite 4.39 -42.43 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.71 -7.71 -8.42 CaCO3

Celestite -2.28 -8.90 -6.62 SrSO4

Chalcedony -0.34 -4.04 -3.70 SiO2

Chlorite(14A) -0.41 72.63 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -4.43 29.32 33.75 Mg3Si2O5(OH)4

CO2(g) -2.43 -3.74 -1.31 CO2

Dolomite 0.93 -15.87 -16.80 CaMg(CO3)2

Gibbsite 2.40 11.21 8.81 Al(OH)3

Gypsum -1.96 -6.55 -4.59 CaSO4:2H2O

H2(g) -41.15 -44.24 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.57 -8.02 1.55 NaCl

Illite 3.32 -38.63 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -0.45 -21.97 -21.52 KAlSi3O8

K-mica 9.89 24.42 14.53 KAl3Si3O10(OH)2

Kaolinite 5.82 14.34 8.52 Al2Si2O5(OH)4

O2(g) -5.14 -7.93 -2.79 O2

Quartz 0.13 -4.04 -4.16 SiO2

Sepiolite -3.27 12.82 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -5.84 12.82 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.22 -4.04 -2.81 SiO2

Strontianite -0.79 -10.07 -9.28 SrCO3

Talc -1.58 21.25 22.82 Mg3Si4O10(OH)2

Witherite -2.67 -11.29 -8.61 BaCO3

Initial solution 27. 09-4-18

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 5.562e-007 5.562e-007

Alkalinity 5.886e-003 5.886e-003

B 1.944e-006 1.944e-006

Ba 6.338e-007 6.338e-007

Ca 2.219e-003 2.219e-003

Cl 6.152e-005 6.152e-005

K 1.126e-005 1.126e-005

Li 5.191e-006 5.191e-006

Mg 7.654e-004 7.654e-004

Na 1.845e-004 1.845e-004

S(6) 1.956e-004 1.956e-004

Si 8.326e-005 8.326e-005

Sr 9.706e-006 9.706e-006

----------------------------Description of solution----------------------------

pH = 7.798 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 414

Density (g/cm3) = 0.99979

Activity of water = 1.000

Ionic strength = 9.012e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.063e-003

Total CO2 (mol/kg) = 6.063e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -1.465e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.22

Iterations = 11

Total H = 1.110186e+002

Total O = 5.552531e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 2.636e-007 2.389e-007 -6.579 -6.622 -0.043

H+ 1.733e-008 1.592e-008 -7.761 -7.798 -0.037

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 5.562e-007

Al(OH)4- 5.500e-007 4.993e-007 -6.260 -6.302 -0.042

Al(OH)3 4.746e-009 4.755e-009 -8.324 -8.323 0.001

Al(OH)2+ 1.476e-009 1.340e-009 -8.831 -8.873 -0.042

AlOH+2 1.236e-011 8.397e-012 -10.908 -11.076 -0.168

Al+3 6.466e-014 2.998e-014 -13.189 -13.523 -0.334

AlSO4+ 9.641e-015 8.753e-015 -14.016 -14.058 -0.042

Al(SO4)2- 3.123e-017 2.835e-017 -16.505 -16.547 -0.042

AlHSO4+2 1.668e-023 1.133e-023 -22.778 -22.946 -0.168

B 1.944e-006

H3BO3 1.884e-006 1.888e-006 -5.725 -5.724 0.001

H2BO3- 5.984e-008 5.433e-008 -7.223 -7.265 -0.042

Ba 6.338e-007

Ba+2 5.945e-007 4.073e-007 -6.226 -6.390 -0.164

BaSO4 2.211e-008 2.216e-008 -7.655 -7.654 0.001

BaHCO3+ 1.525e-008 1.384e-008 -7.817 -7.859 -0.042

BaCO3 1.897e-009 1.901e-009 -8.722 -8.721 0.001

BaOH+ 9.549e-013 8.669e-013 -12.020 -12.062 -0.042

C(4) 6.063e-003

HCO3- 5.680e-003 5.172e-003 -2.246 -2.286 -0.041

CO2 2.241e-004 2.245e-004 -3.650 -3.649 0.001

CaHCO3+ 8.196e-005 7.464e-005 -4.086 -4.127 -0.041

MgHCO3+ 3.194e-005 2.900e-005 -4.496 -4.538 -0.042

CaCO3 2.303e-005 2.308e-005 -4.638 -4.637 0.001

CO3-2 1.671e-005 1.149e-005 -4.777 -4.940 -0.163

MgCO3 4.530e-006 4.539e-006 -5.344 -5.343 0.001

NaHCO3 4.852e-007 4.862e-007 -6.314 -6.313 0.001

SrHCO3+ 3.647e-007 3.321e-007 -6.438 -6.479 -0.041

SrCO3 3.252e-008 3.259e-008 -7.488 -7.487 0.001

NaCO3- 2.097e-008 1.904e-008 -7.678 -7.720 -0.042

BaHCO3+ 1.525e-008 1.384e-008 -7.817 -7.859 -0.042

BaCO3 1.897e-009 1.901e-009 -8.722 -8.721 0.001

Ca 2.219e-003

Ca+2 2.087e-003 1.434e-003 -2.681 -2.843 -0.163

CaHCO3+ 8.196e-005 7.464e-005 -4.086 -4.127 -0.041

CaSO4 2.759e-005 2.764e-005 -4.559 -4.558 0.001

CaCO3 2.303e-005 2.308e-005 -4.638 -4.637 0.001

CaOH+ 1.647e-008 1.495e-008 -7.783 -7.825 -0.042

CaHSO4+ 2.489e-012 2.260e-012 -11.604 -11.646 -0.042

Cl 6.152e-005

Cl- 6.152e-005 5.577e-005 -4.211 -4.254 -0.043

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -44.093 -44.092 0.001

K 1.126e-005

K+ 1.125e-005 1.020e-005 -4.949 -4.991 -0.043

KSO4- 6.890e-009 6.255e-009 -8.162 -8.204 -0.042

KOH 2.217e-012 2.222e-012 -11.654 -11.653 0.001

Li 5.191e-006

Li+ 5.188e-006 4.732e-006 -5.285 -5.325 -0.040

LiSO4- 2.470e-009 2.242e-009 -8.607 -8.649 -0.042

LiOH 6.795e-012 6.810e-012 -11.168 -11.167 0.001

Mg 7.654e-004

Mg+2 7.198e-004 4.976e-004 -3.143 -3.303 -0.160

MgHCO3+ 3.194e-005 2.900e-005 -4.496 -4.538 -0.042

MgSO4 9.158e-006 9.177e-006 -5.038 -5.037 0.001

MgCO3 4.530e-006 4.539e-006 -5.344 -5.343 0.001

MgOH+ 4.042e-008 3.670e-008 -7.393 -7.435 -0.042

Na 1.845e-004

Na+ 1.839e-004 1.672e-004 -3.735 -3.777 -0.042

NaHCO3 4.852e-007 4.862e-007 -6.314 -6.313 0.001

NaSO4- 9.254e-008 8.402e-008 -7.034 -7.076 -0.042

NaCO3- 2.097e-008 1.904e-008 -7.678 -7.720 -0.042

NaOH 6.923e-011 6.938e-011 -10.160 -10.159 0.001

O(0) 1.173e-008

O2 5.867e-009 5.879e-009 -8.232 -8.231 0.001

S(6) 1.956e-004

SO4-2 1.586e-004 1.086e-004 -3.800 -3.964 -0.165

CaSO4 2.759e-005 2.764e-005 -4.559 -4.558 0.001

MgSO4 9.158e-006 9.177e-006 -5.038 -5.037 0.001

SrSO4 1.154e-007 1.157e-007 -6.938 -6.937 0.001

NaSO4- 9.254e-008 8.402e-008 -7.034 -7.076 -0.042

BaSO4 2.211e-008 2.216e-008 -7.655 -7.654 0.001

KSO4- 6.890e-009 6.255e-009 -8.162 -8.204 -0.042

LiSO4- 2.470e-009 2.242e-009 -8.607 -8.649 -0.042

HSO4- 1.443e-010 1.311e-010 -9.841 -9.883 -0.042

CaHSO4+ 2.489e-012 2.260e-012 -11.604 -11.646 -0.042

AlSO4+ 9.641e-015 8.753e-015 -14.016 -14.058 -0.042

Al(SO4)2- 3.123e-017 2.835e-017 -16.505 -16.547 -0.042

AlHSO4+2 1.668e-023 1.133e-023 -22.778 -22.946 -0.168

Si 8.326e-005

H4SiO4 8.272e-005 8.289e-005 -4.082 -4.081 0.001

H3SiO4- 5.382e-007 4.887e-007 -6.269 -6.311 -0.042

H2SiO4-2 1.328e-012 9.020e-013 -11.877 -12.045 -0.168

Sr 9.706e-006

Sr+2 9.193e-006 6.330e-006 -5.037 -5.199 -0.162

SrHCO3+ 3.647e-007 3.321e-007 -6.438 -6.479 -0.041

SrSO4 1.154e-007 1.157e-007 -6.938 -6.937 0.001

SrCO3 3.252e-008 3.259e-008 -7.488 -7.487 0.001

SrOH+ 2.242e-011 2.039e-011 -10.649 -10.690 -0.041

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -1.74 9.87 11.61 Al(OH)3

Albite -3.52 -22.32 -18.80 NaAlSi3O8

Alunite -6.85 -6.70 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.47 -6.81 -4.33 CaSO4

Anorthite -3.54 -23.61 -20.07 CaAl2Si2O8

Aragonite 0.49 -7.78 -8.27 CaCO3

Barite -0.17 -10.35 -10.18 BaSO4

Ca-Montmorillonite 1.09 -45.73 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.64 -7.78 -8.42 CaCO3

Celestite -2.54 -9.16 -6.62 SrSO4

Chalcedony -0.38 -4.08 -3.70 SiO2

Chlorite(14A) -4.07 68.96 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -5.03 28.72 33.75 Mg3Si2O5(OH)4

CO2(g) -2.34 -3.65 -1.31 CO2

Dolomite 0.77 -16.03 -16.80 CaMg(CO3)2

Gibbsite 1.06 9.87 8.81 Al(OH)3

Gypsum -2.22 -6.81 -4.59 CaSO4:2H2O

H2(g) -41.00 -44.09 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.58 -8.03 1.55 NaCl

Illite -0.01 -41.96 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -2.02 -23.54 -21.52 KAlSi3O8

K-mica 5.65 20.18 14.53 KAl3Si3O10(OH)2

Kaolinite 3.06 11.58 8.52 Al2Si2O5(OH)4

O2(g) -5.44 -8.23 -2.79 O2

Quartz 0.08 -4.08 -4.16 SiO2

Sepiolite -3.75 12.34 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -6.32 12.34 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.27 -4.08 -2.81 SiO2

Strontianite -0.86 -10.14 -9.28 SrCO3

Talc -2.27 20.55 22.82 Mg3Si4O10(OH)2

Witherite -2.72 -11.33 -8.61 BaCO3

Initial solution 28. 09-5-20

-----------------------------Solution composition------------------------------

Elements Molality Moles

Alkalinity 6.165e-003 6.165e-003

B 2.406e-006 2.406e-006

Ba 6.702e-007 6.702e-007

Ca 2.282e-003 2.282e-003

Cl 5.616e-005 5.616e-005

K 1.279e-005 1.279e-005

Li 5.191e-006 5.191e-006

Mg 7.860e-004 7.860e-004

N(5) 2.143e-006 2.143e-006

Na 2.041e-004 2.041e-004

S(6) 2.013e-004 2.013e-004

Si 8.992e-005 8.992e-005

Sr 1.062e-005 1.062e-005

----------------------------Description of solution----------------------------

pH = 7.590 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 429

Density (g/cm3) = 0.99981

Activity of water = 1.000

Ionic strength = 9.338e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 6.516e-003

Total CO2 (mol/kg) = 6.516e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -2.462e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.96

Iterations = 9

Total H = 1.110189e+002

Total O = 5.552656e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 1.635e-007 1.479e-007 -6.787 -6.830 -0.043

H+ 2.803e-008 2.571e-008 -7.552 -7.590 -0.038

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

B 2.406e-006

H3BO3 2.360e-006 2.365e-006 -5.627 -5.626 0.001

H2BO3- 4.649e-008 4.214e-008 -7.333 -7.375 -0.043

Ba 6.702e-007

Ba+2 6.284e-007 4.279e-007 -6.202 -6.369 -0.167

BaSO4 2.370e-008 2.375e-008 -7.625 -7.624 0.001

BaHCO3+ 1.687e-008 1.530e-008 -7.773 -7.815 -0.043

BaCO3 1.298e-009 1.300e-009 -8.887 -8.886 0.001

BaOH+ 6.221e-013 5.640e-013 -12.206 -12.249 -0.043

C(4) 6.516e-003

HCO3- 5.982e-003 5.440e-003 -2.223 -2.264 -0.041

CO2 3.806e-004 3.814e-004 -3.420 -3.419 0.001

CaHCO3+ 8.840e-005 8.039e-005 -4.054 -4.095 -0.041

MgHCO3+ 3.436e-005 3.115e-005 -4.464 -4.507 -0.043

CaCO3 1.536e-005 1.539e-005 -4.814 -4.813 0.001

CO3-2 1.094e-005 7.484e-006 -4.961 -5.126 -0.165

MgCO3 3.012e-006 3.018e-006 -5.521 -5.520 0.001

NaHCO3 5.635e-007 5.647e-007 -6.249 -6.248 0.001

SrHCO3+ 4.176e-007 3.797e-007 -6.379 -6.421 -0.041

SrCO3 2.302e-008 2.307e-008 -7.638 -7.637 0.001

BaHCO3+ 1.687e-008 1.530e-008 -7.773 -7.815 -0.043

NaCO3- 1.511e-008 1.369e-008 -7.821 -7.863 -0.043

BaCO3 1.298e-009 1.300e-009 -8.887 -8.886 0.001

Ca 2.282e-003

Ca+2 2.149e-003 1.469e-003 -2.668 -2.833 -0.165

CaHCO3+ 8.840e-005 8.039e-005 -4.054 -4.095 -0.041

CaSO4 2.881e-005 2.887e-005 -4.540 -4.540 0.001

CaCO3 1.536e-005 1.539e-005 -4.814 -4.813 0.001

CaOH+ 1.046e-008 9.481e-009 -7.981 -8.023 -0.043

CaHSO4+ 4.205e-012 3.812e-012 -11.376 -11.419 -0.043

Cl 5.616e-005

Cl- 5.616e-005 5.083e-005 -4.251 -4.294 -0.043

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.677 -43.676 0.001

K 1.279e-005

K+ 1.279e-005 1.157e-005 -4.893 -4.937 -0.043

KSO4- 7.984e-009 7.238e-009 -8.098 -8.140 -0.043

KOH 1.557e-012 1.560e-012 -11.808 -11.807 0.001

Li 5.191e-006

Li+ 5.188e-006 4.725e-006 -5.285 -5.326 -0.041

LiSO4- 2.519e-009 2.284e-009 -8.599 -8.641 -0.043

LiOH 4.201e-012 4.210e-012 -11.377 -11.376 0.001

Mg 7.860e-004

Mg+2 7.391e-004 5.081e-004 -3.131 -3.294 -0.163

MgHCO3+ 3.436e-005 3.115e-005 -4.464 -4.507 -0.043

MgSO4 9.537e-006 9.557e-006 -5.021 -5.020 0.001

MgCO3 3.012e-006 3.018e-006 -5.521 -5.520 0.001

MgOH+ 2.559e-008 2.320e-008 -7.592 -7.634 -0.043

N(5) 2.143e-006

NO3- 2.143e-006 1.936e-006 -5.669 -5.713 -0.044

Na 2.041e-004

Na+ 2.034e-004 1.846e-004 -3.692 -3.734 -0.042

NaHCO3 5.635e-007 5.647e-007 -6.249 -6.248 0.001

NaSO4- 1.044e-007 9.463e-008 -6.981 -7.024 -0.043

NaCO3- 1.511e-008 1.369e-008 -7.821 -7.863 -0.043

NaOH 4.733e-011 4.744e-011 -10.325 -10.324 0.001

O(0) 1.724e-009

O2 8.619e-010 8.638e-010 -9.065 -9.064 0.001

S(6) 2.013e-004

SO4-2 1.627e-004 1.107e-004 -3.789 -3.956 -0.167

CaSO4 2.881e-005 2.887e-005 -4.540 -4.540 0.001

MgSO4 9.537e-006 9.557e-006 -5.021 -5.020 0.001

SrSO4 1.279e-007 1.282e-007 -6.893 -6.892 0.001

NaSO4- 1.044e-007 9.463e-008 -6.981 -7.024 -0.043

BaSO4 2.370e-008 2.375e-008 -7.625 -7.624 0.001

KSO4- 7.984e-009 7.238e-009 -8.098 -8.140 -0.043

LiSO4- 2.519e-009 2.284e-009 -8.599 -8.641 -0.043

HSO4- 2.381e-010 2.159e-010 -9.623 -9.666 -0.043

CaHSO4+ 4.205e-012 3.812e-012 -11.376 -11.419 -0.043

Si 8.992e-005

H4SiO4 8.956e-005 8.975e-005 -4.048 -4.047 0.001

H3SiO4- 3.614e-007 3.276e-007 -6.442 -6.485 -0.043

H2SiO4-2 5.544e-013 3.744e-013 -12.256 -12.427 -0.171

Sr 1.062e-005

Sr+2 1.005e-005 6.882e-006 -4.998 -5.162 -0.165

SrHCO3+ 4.176e-007 3.797e-007 -6.379 -6.421 -0.041

SrSO4 1.279e-007 1.282e-007 -6.893 -6.892 0.001

SrCO3 2.302e-008 2.307e-008 -7.638 -7.637 0.001

SrOH+ 1.511e-011 1.373e-011 -10.821 -10.862 -0.042

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Anhydrite -2.45 -6.79 -4.33 CaSO4

Aragonite 0.31 -7.96 -8.27 CaCO3

Barite -0.14 -10.32 -10.18 BaSO4

Calcite 0.46 -7.96 -8.42 CaCO3

Celestite -2.49 -9.12 -6.62 SrSO4

Chalcedony -0.35 -4.05 -3.70 SiO2

Chrysotile -6.18 27.56 33.75 Mg3Si2O5(OH)4

CO2(g) -2.11 -3.42 -1.31 CO2

Dolomite 0.42 -16.38 -16.80 CaMg(CO3)2

Gypsum -2.20 -6.79 -4.59 CaSO4:2H2O

H2(g) -40.58 -43.68 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.58 -8.03 1.55 NaCl

O2(g) -6.27 -9.06 -2.79 O2

Quartz 0.12 -4.05 -4.16 SiO2

Sepiolite -4.46 11.63 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -7.03 11.63 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.23 -4.05 -2.81 SiO2

Strontianite -1.01 -10.29 -9.28 SrCO3

Talc -3.35 19.47 22.82 Mg3Si4O10(OH)2

Witherite -2.88 -11.49 -8.61 BaCO3

Initial solution 29. 09-7-7

-----------------------------Solution composition------------------------------

Elements Molality Moles

Al 1.669e-006 1.669e-006

Alkalinity 6.428e-003 6.428e-003

B 3.054e-006 3.054e-006

Ba 6.120e-007 6.120e-007

Ca 2.329e-003 2.329e-003

Cl 7.055e-005 7.055e-005

K 1.459e-005 1.459e-005

Li 5.624e-006 5.624e-006

Mg 9.301e-004 9.301e-004

N(5) 1.714e-006 1.714e-006

Na 2.468e-004 2.468e-004

S(6) 2.898e-004 2.898e-004

Si 1.011e-004 1.011e-004

Sr 1.405e-005 1.405e-005

----------------------------Description of solution----------------------------

pH = 7.290 Equilibrium with Calcite

pe = 12.700

Specific Conductance (uS/cm, 13 oC) = 457

Density (g/cm3) = 0.99983

Activity of water = 1.000

Ionic strength = 9.984e-003

Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 7.197e-003

Total CO2 (mol/kg) = 7.197e-003

Temperature (deg C) = 13.000

Electrical balance (eq) = -2.598e-004

Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -1.95

Iterations = 11

Total H = 1.110192e+002

Total O = 5.552860e+001

----------------------------Distribution of species----------------------------

Log Log Log

Species Molality Activity Molality Activity Gamma

OH- 8.220e-008 7.414e-008 -7.085 -7.130 -0.045

H+ 5.605e-008 5.128e-008 -7.251 -7.290 -0.039

H2O 5.551e+001 9.998e-001 1.744 -0.000 0.000

Al 1.669e-006

Al(OH)4- 1.580e-006 1.428e-006 -5.801 -5.845 -0.044

Al(OH)2+ 4.403e-008 3.979e-008 -7.356 -7.400 -0.044

Al(OH)3 4.372e-008 4.382e-008 -7.359 -7.358 0.001

AlOH+2 1.203e-009 8.032e-010 -8.920 -9.095 -0.176

Al+3 2.056e-011 9.241e-012 -10.687 -11.034 -0.347

AlSO4+ 4.303e-012 3.889e-012 -11.366 -11.410 -0.044

Al(SO4)2- 2.009e-014 1.816e-014 -13.697 -13.741 -0.044

AlHSO4+2 2.430e-020 1.622e-020 -19.614 -19.790 -0.176

B 3.054e-006

H3BO3 3.024e-006 3.031e-006 -5.519 -5.518 0.001

H2BO3- 2.996e-008 2.708e-008 -7.524 -7.567 -0.044

Ba 6.120e-007

Ba+2 5.658e-007 3.810e-007 -6.247 -6.419 -0.172

BaSO4 2.982e-008 2.989e-008 -7.526 -7.525 0.001

BaHCO3+ 1.571e-008 1.420e-008 -7.804 -7.848 -0.044

BaCO3 6.037e-010 6.051e-010 -9.219 -9.218 0.001

BaOH+ 2.785e-013 2.517e-013 -12.555 -12.599 -0.044

C(4) 7.197e-003

HCO3- 6.253e-003 5.671e-003 -2.204 -2.246 -0.042

CO2 7.913e-004 7.931e-004 -3.102 -3.101 0.001

CaHCO3+ 9.301e-005 8.435e-005 -4.031 -4.074 -0.042

MgHCO3+ 4.187e-005 3.784e-005 -4.378 -4.422 -0.044

CaCO3 8.076e-006 8.094e-006 -5.093 -5.092 0.001

CO3-2 5.783e-006 3.911e-006 -5.238 -5.408 -0.170

MgCO3 1.834e-006 1.838e-006 -5.737 -5.736 0.001

NaHCO3 7.079e-007 7.095e-007 -6.150 -6.149 0.001

SrHCO3+ 5.682e-007 5.153e-007 -6.246 -6.288 -0.042

BaHCO3+ 1.571e-008 1.420e-008 -7.804 -7.848 -0.044

SrCO3 1.566e-008 1.569e-008 -7.805 -7.804 0.001

NaCO3- 9.542e-009 8.624e-009 -8.020 -8.064 -0.044

BaCO3 6.037e-010 6.051e-010 -9.219 -9.218 0.001

Ca 2.329e-003

Ca+2 2.187e-003 1.478e-003 -2.660 -2.830 -0.170

CaHCO3+ 9.301e-005 8.435e-005 -4.031 -4.074 -0.042

CaSO4 4.098e-005 4.108e-005 -4.387 -4.386 0.001

CaCO3 8.076e-006 8.094e-006 -5.093 -5.092 0.001

CaOH+ 5.293e-009 4.784e-009 -8.276 -8.320 -0.044

CaHSO4+ 1.197e-011 1.082e-011 -10.922 -10.966 -0.044

Cl 7.055e-005

Cl- 7.055e-005 6.366e-005 -4.151 -4.196 -0.045

H(0) 0.000e+000

H2 0.000e+000 0.000e+000 -43.077 -43.076 0.001

K 1.459e-005

K+ 1.457e-005 1.315e-005 -4.836 -4.881 -0.045

KSO4- 1.286e-008 1.162e-008 -7.891 -7.935 -0.044

KOH 8.868e-013 8.889e-013 -12.052 -12.051 0.001

Li 5.624e-006

Li+ 5.620e-006 5.104e-006 -5.250 -5.292 -0.042

LiSO4- 3.858e-009 3.487e-009 -8.414 -8.458 -0.044

LiOH 2.275e-012 2.280e-012 -11.643 -11.642 0.001

Mg 9.301e-004

Mg+2 8.707e-004 5.923e-004 -3.060 -3.227 -0.167

MgHCO3+ 4.187e-005 3.784e-005 -4.378 -4.422 -0.044

MgSO4 1.571e-005 1.575e-005 -4.804 -4.803 0.001

MgCO3 1.834e-006 1.838e-006 -5.737 -5.736 0.001

MgOH+ 1.500e-008 1.356e-008 -7.824 -7.868 -0.044

N(5) 1.714e-006

NO3- 1.714e-006 1.544e-006 -5.766 -5.811 -0.045

Na 2.468e-004

Na+ 2.459e-004 2.225e-004 -3.609 -3.653 -0.043

NaHCO3 7.079e-007 7.095e-007 -6.150 -6.149 0.001

NaSO4- 1.783e-007 1.612e-007 -6.749 -6.793 -0.044

NaCO3- 9.542e-009 8.624e-009 -8.020 -8.064 -0.044

NaOH 2.859e-011 2.866e-011 -10.544 -10.543 0.001

O(0) 1.089e-010

O2 5.443e-011 5.455e-011 -10.264 -10.263 0.001

S(6) 2.898e-004

SO4-2 2.326e-004 1.565e-004 -3.633 -3.805 -0.172

CaSO4 4.098e-005 4.108e-005 -4.387 -4.386 0.001

MgSO4 1.571e-005 1.575e-005 -4.804 -4.803 0.001

SrSO4 2.354e-007 2.359e-007 -6.628 -6.627 0.001

NaSO4- 1.783e-007 1.612e-007 -6.749 -6.793 -0.044

BaSO4 2.982e-008 2.989e-008 -7.526 -7.525 0.001

KSO4- 1.286e-008 1.162e-008 -7.891 -7.935 -0.044

LiSO4- 3.858e-009 3.487e-009 -8.414 -8.458 -0.044

HSO4- 6.734e-010 6.087e-010 -9.172 -9.216 -0.044

CaHSO4+ 1.197e-011 1.082e-011 -10.922 -10.966 -0.044

AlSO4+ 4.303e-012 3.889e-012 -11.366 -11.410 -0.044

Al(SO4)2- 2.009e-014 1.816e-014 -13.697 -13.741 -0.044

AlHSO4+2 2.430e-020 1.622e-020 -19.614 -19.790 -0.176

Si 1.011e-004

H4SiO4 1.009e-004 1.011e-004 -3.996 -3.995 0.001

H3SiO4- 2.047e-007 1.850e-007 -6.689 -6.733 -0.044

H2SiO4-2 1.588e-013 1.060e-013 -12.799 -12.975 -0.176

Sr 1.405e-005

Sr+2 1.323e-005 8.957e-006 -4.879 -5.048 -0.169

SrHCO3+ 5.682e-007 5.153e-007 -6.246 -6.288 -0.042

SrSO4 2.354e-007 2.359e-007 -6.628 -6.627 0.001

SrCO3 1.566e-008 1.569e-008 -7.805 -7.804 0.001

SrOH+ 9.887e-012 8.957e-012 -11.005 -11.048 -0.043

------------------------------Saturation indices-------------------------------

Phase SI log IAP log KT

Al(OH)3(a) -0.78 10.84 11.61 Al(OH)3

Albite -2.69 -21.48 -18.80 NaAlSi3O8

Alunite -2.00 -1.86 0.14 KAl3(SO4)2(OH)6

Anhydrite -2.30 -6.64 -4.33 CaSO4

Anorthite -2.44 -22.51 -20.07 CaAl2Si2O8

Aragonite 0.03 -8.24 -8.27 CaCO3

Barite -0.04 -10.22 -10.18 BaSO4

Ca-Montmorillonite 3.49 -43.33 -46.82 Ca0.165Al2.33Si3.67O10(OH)2

Calcite 0.18 -8.24 -8.42 CaCO3

Celestite -2.23 -8.85 -6.62 SrSO4

Chalcedony -0.30 -4.00 -3.70 SiO2

Chlorite(14A) -6.59 66.45 73.04 Mg5Al2Si3O10(OH)8

Chrysotile -7.68 26.07 33.75 Mg3Si2O5(OH)4

CO2(g) -1.79 -3.10 -1.31 CO2

Dolomite -0.07 -16.87 -16.80 CaMg(CO3)2

Gibbsite 2.02 10.84 8.81 Al(OH)3

Gypsum -2.05 -6.64 -4.59 CaSO4:2H2O

H2(g) -39.98 -43.08 -3.10 H2

H2O(g) -1.83 -0.00 1.83 H2O

Halite -9.40 -7.85 1.55 NaCl

Illite 2.04 -39.91 -41.95 K0.6Mg0.25Al2.3Si3.5O10(OH)2

K-feldspar -1.19 -22.71 -21.52 KAlSi3O8

K-mica 8.40 22.93 14.53 KAl3Si3O10(OH)2

Kaolinite 5.16 13.68 8.52 Al2Si2O5(OH)4

O2(g) -7.47 -10.26 -2.79 O2

Quartz 0.17 -4.00 -4.16 SiO2

Sepiolite -5.37 10.72 16.09 Mg2Si3O7.5OH:3H2O

Sepiolite(d) -7.94 10.72 18.66 Mg2Si3O7.5OH:3H2O

SiO2(a) -1.18 -4.00 -2.81 SiO2

Strontianite -1.18 -10.46 -9.28 SrCO3

Talc -4.75 18.08 22.82 Mg3Si4O10(OH)2

Witherite -3.22 -11.83 -8.61 BaCO3

------------------

End of simulation.

------------------

------------------------------------

Reading input data for simulation 2.

------------------------------------

-----------

End of run.

-----------