

Appendix A. Carbonate Precipitation Simulated at Surface Conditions

Table A-1 Control vessels incubated under 40 °C and 15 psi

Sample Name	Incubation days	T*	P	pH	Alkalinity	Mg ²⁺	Ca ²⁺	Mg:Ca ratio	Charge Balance	SI_Dolomite	SI_Calcite	SI_Aragonite	mol% MgCO ₃ in solids
Initial Solution	0	40	15	8.2	2.74	58.00	38.00	1.53	1.39%	3.33	1.44	1.3	
Sil_Dec19_cc0	0.5	40	15	8.2	0.80	55.05	35.98	1.53	0.9%	2.19	0.85	0.71	11.61
Sil_Dec19_cc1	1	40	15	7.79	0.69	52.30	33.99	1.54	0.2%	1.16	0.33	0.2	11.57
Sil_Dec19_cc2	2	40	15	7.75	0.82	56.68	37.22	1.52	1.32%	1.58	0.54	0.41	11.55
Sil_Dec19_cc3	5	40	15	7.6	0.88	59.77	39.34	1.52	2.07%	1.42	0.46	0.33	11.56
Sil_Dec19_cc4	10	40	15	7.53	0.66	59.50	39.15	1.52	2.02%	1.04	0.27	0.14	11.54
Sil_Dec19_cc5	15	40	15	7.63	0.60	58.65	38.58	1.52	1.82%	1.12	0.31	0.18	11.58
Sil_Dec19_cc6	20	40	15	7.565	0.63	60.52	39.80	1.52	2.26%	1.08	0.29	0.16	11.52
Sil_Dec19_cc7	25	40	15	7.55	0.65	59.67	39.37	1.52	2.07%	1.06	0.28	0.15	11.53
Sil_Dec19_cc8	30	40	15	7.515	0.70	65.37	42.79	1.53	3.37%	1.13	0.31	0.18	11.53
Sil_Dec19_cc9	80	40	15	7.46	0.62	67.05	44.24	1.52	3.81%	0.93	0.22	0.08	11.55
Sil_July02_cc	121	40	15	7.53	0.48	48.90	34.17	1.43	0.39%	-2.15	-1.31	-1.44	11.55

* Units for T, P and all aqueous concentrations are °C, psi and mmol L⁻¹, respectively.

Table A-2 Experimental vessels** incubated under 40 °C and 15 psi

Name	Incubation days	T*	P	pH	Alkalinity	Mg ²⁺	Ca ²⁺	Mg:Ca ratio	Charge Balance	SI_Dolomite	SI_Calcite	SI_Aragonite	mol% MgCO ₃ in solids
Initial Solution	0	40	15	8.2	0.80	58.00	38.00	1.53	1.39%	3.33	1.44	1.3	
Sil_Dec19_sp0	0.5	40	15	8.2	0.80	55.13	35.98	1.53	0.91%	2.19	0.85	0.71	11.61
Sil_Dec19_sp1	1	40	15	7.62	0.83	55.04	36.02	1.53	0.9%	1.21	0.35	0.22	11.53
Sil_Dec19_sp2	2	40	15	7.625	0.71	56.58	37.02	1.53	1.28%	1.24	0.37	0.24	11.54
Sil_Dec19_sp3	5	40	15	7.72	0.68	57.73	37.76	1.53	1.56%	1.36	0.43	0.3	11.53
Sil_Dec19_sp4	10	40	15	7.75	0.69	61.24	40.24	1.52	2.42%	1.46	0.48	0.35	11.55
Sil_Dec19_sp5	15	40	15	7.635	0.72	60.98	39.97	1.53	2.34%	1.3	0.4	0.27	11.56
Sil_Dec19_sp6	20	40	15	7.56	0.69	58.08	38.40	1.51	1.7%	1.12	0.31	0.18	11.57
Sil_Dec19_sp7	25	40	15	7.56	0.66	57.91	38.29	1.51	1.66%	1.07	0.29	0.15	11.53
Sil_Dec19_sp8	30	40	15	7.505	0.70	59.89	39.71	1.51	2.15%	1.06	0.28	0.15	11.52
Sil_Dec19_sp9	80	40	15	7.56	0.60	67.06	44.28	1.51	3.82%	1.08	0.29	0.16	11.55
Sil_July02_sp	121	40	15	7.4	0.50	49.02	34.26	1.43	0.42%	-2.14	-1.3	-1.44	11.56

* Units for T, P and all aqueous concentrations are °C, psi and mmol L⁻¹, respectively.

** Concentration of 0.82µm COM in experimental vessels is 1×10⁻² mg L⁻¹.

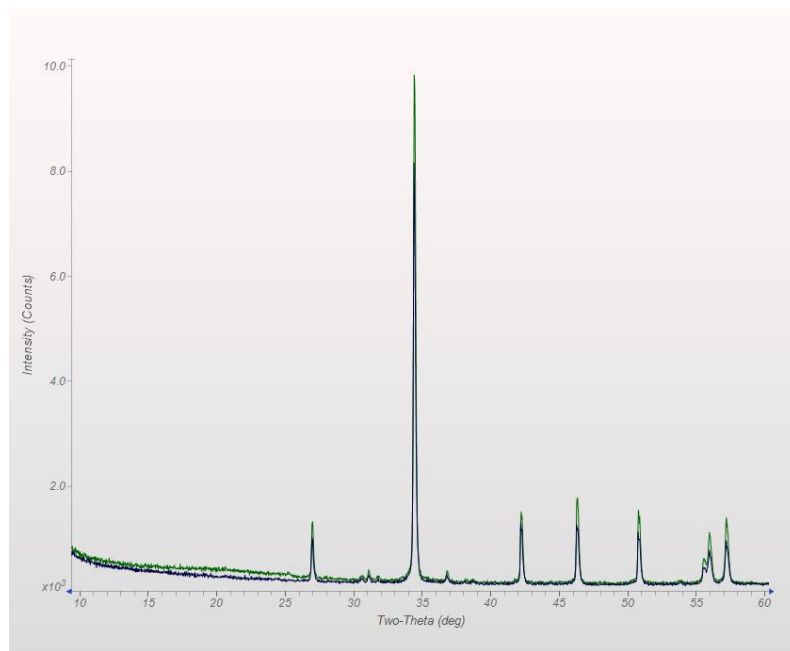


Figure A-1 XRD graph of experimental vessel (green line) and control vessel at 121 d

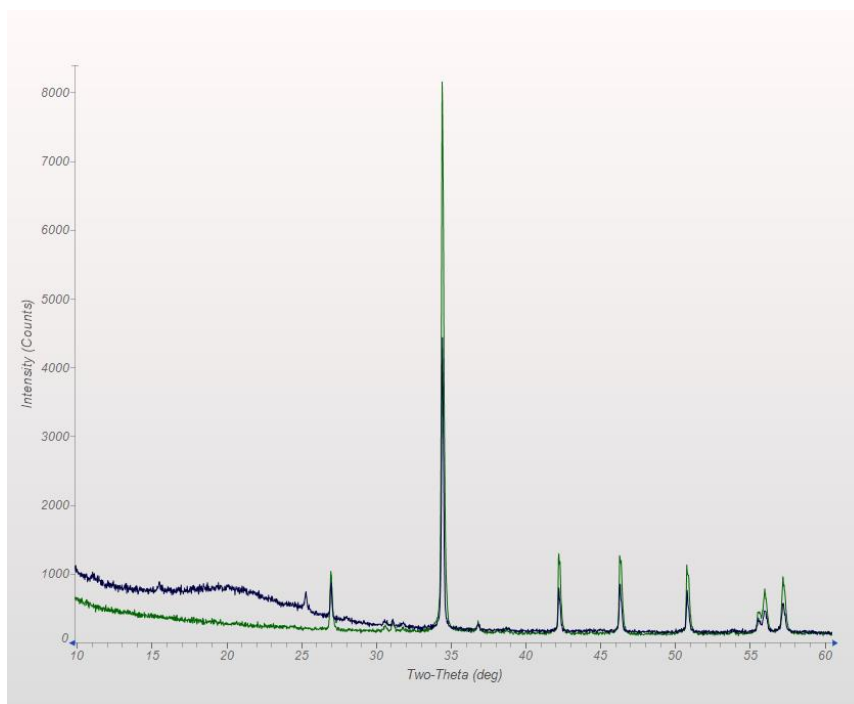


Figure A-2 Control vessels at 15 d and 121 d (Green line)

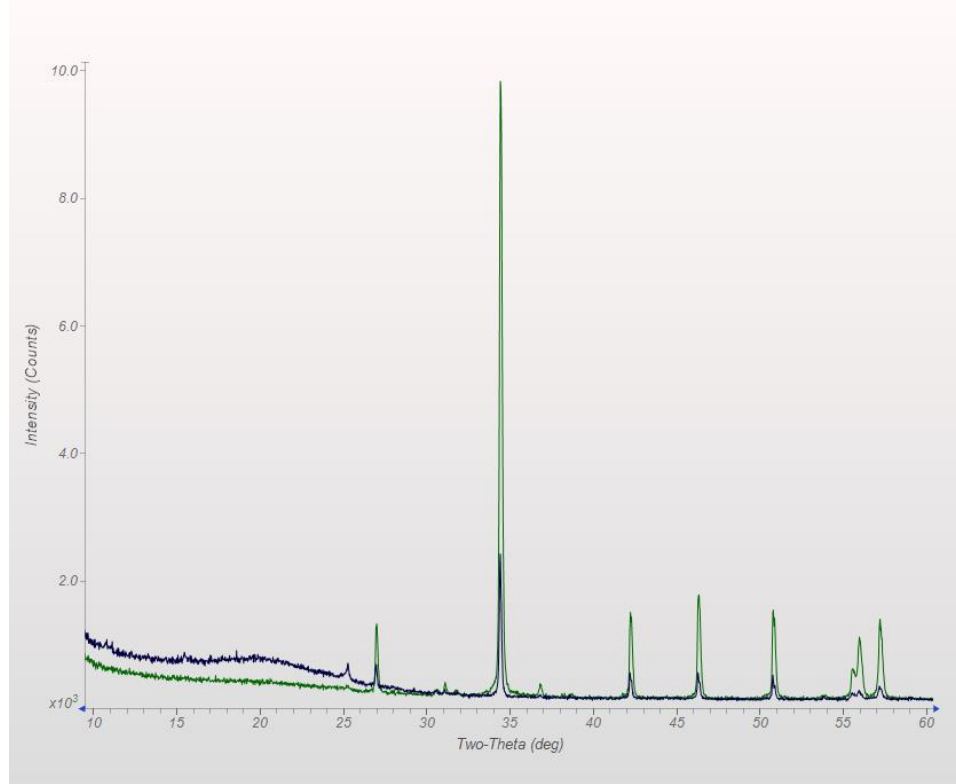


Figure A-3 Experimental vessels at 15 d and 121 d (green line)

Appendix B Experimentally-simulated Diagenesis

Table B-1 Experimental vessels** incubated under increased P and T

Sample Name	Incubation days	T*	P	pH	Alkalinity	Mg ²⁺	Ca ²⁺	Mg:Ca ratio	Charge Balance	SI_Dolomite	SI_Calcite	SI_Aragonite	mol% MgCO ₃ in solids
Sil_Dec19_sp_I	87	40	100	7.54	0.52	61.94	40.86	1.52	2.62%	0.86	0.18	0.05	11.56
Sil_Dec19_sp_II	98	41	160	7.49	0.48	71.22	46.55	1.53	4.72%	0.8	0.14	0.01	11.53
Sil_Dec19_sp_III	105	47.5	900	7.85	0.42	66.49	43.23	1.54	3.61%	1.25	0.35	0.23	11.51

* Units for T, P and all aqueous concentrations are °C, psi and mmol L⁻¹, respectively.

** Concentration of 0.82µm COM in experimental vessels is 1×10⁻² mg L⁻¹.

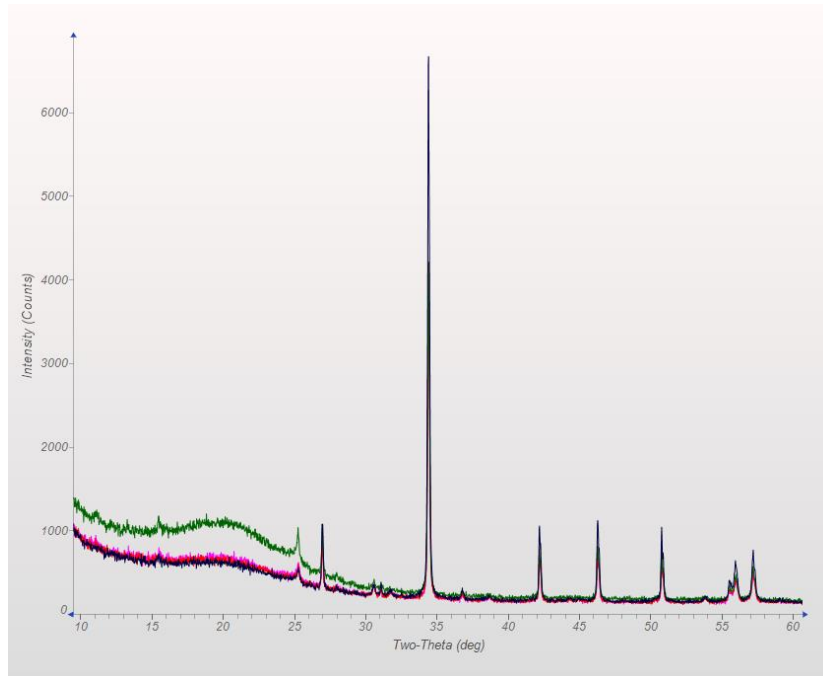


Figure B-1 XRD pattern at 80 d, 87 d (green line), 98d (red line), and 105d(pink line)

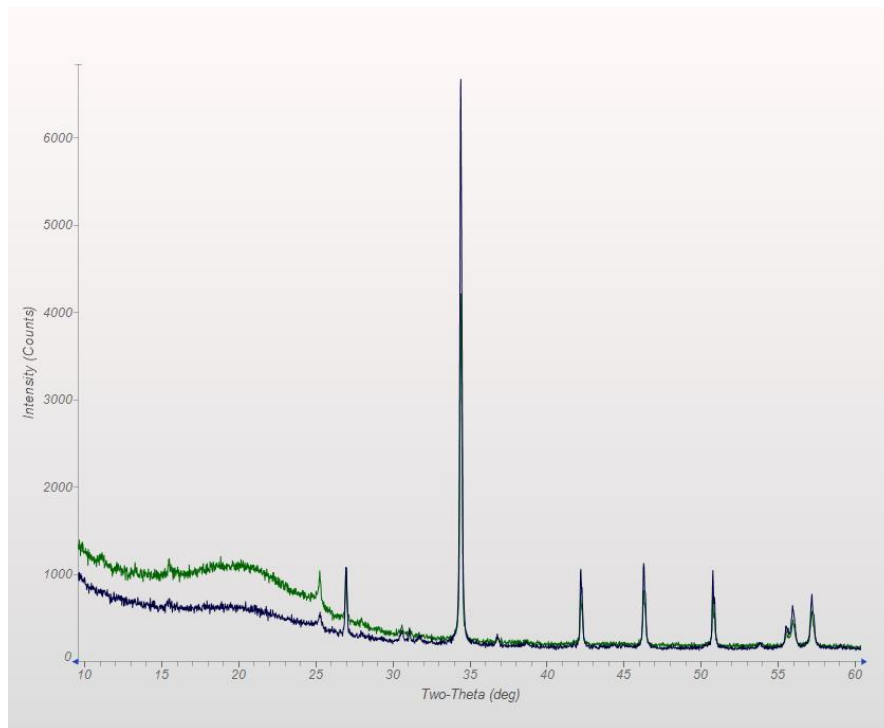


Figure B-2 XRD pattern at 80 d and 87 d (red line)

Appendix C Effect of Pressure on Carbonate Recrystallization

Table C-1 Control vessels incubated under increased P (T fixed at 40 °C)

Sample Name	Incubation days	T*	P	pH	Alkalinity	Mg ²⁺	Ca ²⁺	Mg:Ca ratio	Charge Balance	SI_Dolomite	SI_Calcite	SI_Aragonite	mol% MgCO ₃ solids
Initial Solution	0	40	15	8.2	2.59	51.89	37.84	1.37	2.33%	3.27	1.41	1.28	
May_ID=0.5	0.5	40	15	8.2	1.00	51.67	37.62	1.37	3.12%	2.44	0.99	0.85	11.61
May_ID=14	14	40	15	7.7	0.60	53.09	37.03	1.43	2.67%	1.22	0.37	0.24	11.60
May_ID=14+7	21	40	160	7.69	0.52	48.07	33.12	1.45	1.09%	0.99	0.26	0.13	11.53
May_ID=14+7+5	26	40	200	7.5	0.48	49.78	34.68	1.44	1.64%	0.61	0.07	-0.06	11.53
May_ID=14+7+5+5	31	40	550	7.55	0.36	51.31	36.10	1.42	2.13%	0.44	-0.02	-0.15	11.60
May_ID=14+7+5+5+5	36	40	900	7.9	0.40	49.45	33.82	1.46	1.45%	1.04	0.28	0.15	11.61

* Units for T, P and all aqueous concentrations are °C, psi and mmol L⁻¹, respectively.

Table C-2 Experimental vessels** incubated under increased P (T fixed at 40 °C)

Sample Name	Incubation days	T*	P	pH	Alkalinity	Mg ²⁺	Ca ²⁺	Mg:Ca ratio	Charge Balance	SI_Dolomite	SI_Calcite	SI_Aragonite	mol% MgCO ₃ in solids
Initial Solution	0	40	15	8.2	2.4	48.00	35.00	1.37	1.23%	3.3	1.4	1.3	
Apr_ID=0	0.5	40	15	8.2	1	42.03	30.04	1.40	-0.52%	2.4	1.0	0.9	
Apr_ID=14	14	40	15	7.49	0.92	48.00	34.13	1.41	1.21%	1.2	0.4	0.2	11.56
Apr_ID=14+7	21	40	160	7.54	0.96	43.78	30.85	1.42	-0.07%	1.0	0.3	0.1	11.63
Apr_ID=14+7+5	26	40	200	7.50	0.64	50.42	36.31	1.39	2.00%	0.6	0.1	-0.1	
Apr_ID=14+7+5+5	31	40	550	7.72	0.48	48.38	34.11	1.42	1.31%	0.4	0.0	-0.2	11.59
Apr_ID=14+7+5+5+5	36	40	900	7.73	0.4	50.81	35.55	1.43	1.96%	0.63	0.07	-0.06	

* Units for T, P and all aqueous concentrations are °C, psi and mmol L⁻¹, respectively.

** Concentration of 0.82µm COM in experimental vessels is 1×10⁻² mg L⁻¹.

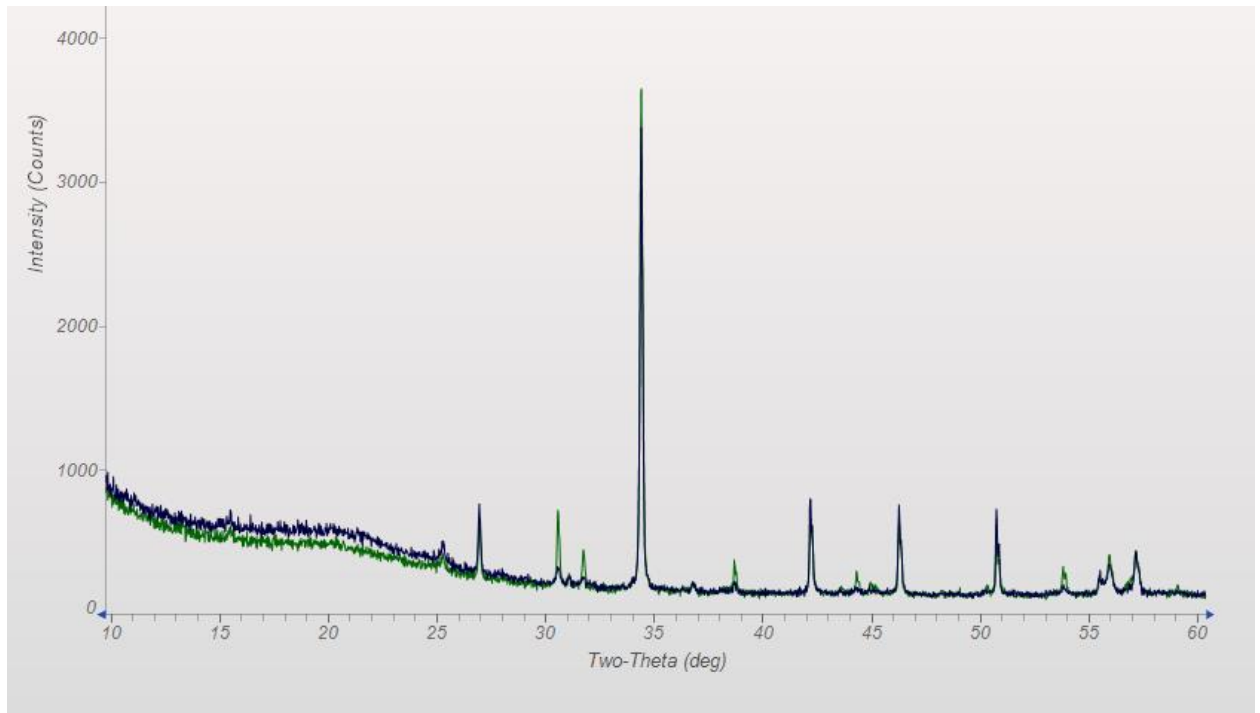


Figure C-1 XRD pattern at 14 d and 31 d (green)

Appendix D Phreeqc Reports

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
 1\Appendix\Recipe_Silurian_PCO2_initial.pqi
 Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
 1\Appendix\Recipe_Silurian_PCO2_initial.pqi
 Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
 15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35.98
Mg 55.13
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 584
water 1 # kg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.598e-02	3.598e-02
Cl	5.840e-01	5.840e-01
Mg	5.513e-02	5.513e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	68923
Density (g/cm^3)	=	1.01702
Volume (L)	=	1.01758
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.967e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.979e-03
Total CO2 (mol/kg)	=	1.979e-03
Temperature (°C)	=	40.00
Electrical balance (eq)	=	1.882e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.55
Iterations	=	7
Total H	=	1.110141e+02
Total O	=	5.555619e+01

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

mole V Species cm ³ /mol	Molality	Activity	Log		Log	
			Molality	Activity	Gamma	
OH-	7.596e-06	4.552e-06	-5.119	-5.342	-0.222	-
2.16						
H+	8.423e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00						
H2O	5.551e+01	9.809e-01	1.744	-0.008	0.000	
18.16						
C(4)	1.979e-03					
HCO3-	1.126e-03	7.519e-04	-2.948	-3.124	-0.176	
27.71						
MgHCO3+	2.224e-04	1.378e-04	-3.653	-3.861	-0.208	
6.16						
CaHCO3+	1.377e-04	9.423e-05	-3.861	-4.026	-0.165	
10.44						
CaCO3	1.227e-04	1.440e-04	-3.911	-3.841	0.070	-
14.56						
NaCO3-	1.158e-04	8.608e-05	-3.936	-4.065	-0.129	
4.23						
MgCO3	1.050e-04	1.232e-04	-3.979	-3.909	0.070	-
17.10						
NaHCO3	1.045e-04	1.226e-04	-3.981	-3.911	0.070	
1.80						
CO3-2	3.604e-05	7.153e-06	-4.443	-5.146	-0.702	-
1.61						
CO2	8.171e-06	9.593e-06	-5.088	-5.018	0.070	
35.16						
(CO2)2	2.266e-12	2.661e-12	-11.645	-11.575	0.070	
70.32						
Ca	3.598e-02					
Ca+2	3.461e-02	8.305e-03	-1.461	-2.081	-0.620	-
16.44						
CaSO4	1.107e-03	1.300e-03	-2.956	-2.886	0.070	
7.96						
CaHCO3+	1.377e-04	9.423e-05	-3.861	-4.026	-0.165	
10.44						
CaCO3	1.227e-04	1.440e-04	-3.911	-3.841	0.070	-
14.56						
CaOH+	2.883e-07	2.142e-07	-6.540	-6.669	-0.129	
(0)						
CaHSO4+	9.209e-11	6.844e-11	-10.036	-10.165	-0.129	
(0)						
Cl	5.840e-01					
Cl-	5.840e-01	3.629e-01	-0.234	-0.440	-0.207	
19.09						
H(0)	4.165e-28					
H2	2.082e-28	2.445e-28	-27.681	-27.612	0.070	
28.59						
Mg	5.513e-02					
Mg+2	5.149e-02	1.434e-02	-1.288	-1.844	-0.555	-
20.79						
MgSO4	3.270e-03	3.839e-03	-2.485	-2.416	0.070	
6.30						

MgHCO3+	2.224e-04	1.378e-04	-3.653	-3.861	-0.208	
6.16						
MgCO3	1.050e-04	1.232e-04	-3.979	-3.909	0.070	-
17.10						
MgOH+	4.214e-05	2.939e-05	-4.375	-4.532	-0.156	
(0)						
Na	4.450e-01					
Na+	4.427e-01	3.145e-01	-0.354	-0.502	-0.149	
0.06						
NaSO4-	2.044e-03	1.364e-03	-2.689	-2.865	-0.176	
21.03						
NaCO3-	1.158e-04	8.608e-05	-3.936	-4.065	-0.129	
4.23						
NaHCO3	1.045e-04	1.226e-04	-3.981	-3.911	0.070	
1.80						
NaOH	1.219e-16	1.431e-16	-15.914	-15.844	0.070	
(0)						
O(0)	4.646e-33					
O2	2.323e-33	2.727e-33	-32.634	-32.564	0.070	
31.40						
S(6)	1.100e-02					
SO4-2	4.579e-03	7.907e-04	-2.339	-3.102	-0.763	
19.26						
MgSO4	3.270e-03	3.839e-03	-2.485	-2.416	0.070	
6.30						
NaSO4-	2.044e-03	1.364e-03	-2.689	-2.865	-0.176	
21.03						
CaSO4	1.107e-03	1.300e-03	-2.956	-2.886	0.070	
7.96						
HSO4-	9.224e-10	6.855e-10	-9.035	-9.164	-0.129	
41.79						
CaHSO4+	9.209e-11	6.844e-11	-10.036	-10.165	-0.129	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.73	-5.18	-4.45	CaSO4
Aragonite	1.22	-7.23	-8.45	CaCO3
Calcite	1.35	-7.23	-8.58	CaCO3
CO2(g)	-3.39	-5.02	-1.63	CO2
Dolomite	3.21	-14.22	-17.42	CaMg(CO3)2
Gypsum	-0.60	-5.20	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.52	-0.94	1.58	NaCl
O2(g)	-29.58	-32.56	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.301 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
1\Appendix\Recipe_Silurian_PCO2_121_sp.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
1\Appendix\Recipe_Silurian_PCO2_121_sp.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.3
pe 4
redox pe
units mmol/kgw
density 1
Ca 34.26
Mg 49.0205
Na 445
S(6) 11
Alkalinity 0.4975 as HCO3-
Cl 584
water 1 # kg
GAS_PHASE 1
fixed_pressure
pressure 1
volume 1
temperature 30
CO2(g) 0.009

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	4.975e-04	4.975e-04
Ca	3.426e-02	3.426e-02
Cl	5.840e-01	5.840e-01
Mg	4.902e-02	4.902e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH = 7.300
pe = 4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C) = 68601
Density (g/cm^3) = 1.01660
Volume (L) = 1.01769
Activity of water = 0.981
Ionic strength (mol/kgw) = 6.822e-01
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 4.976e-04
Total CO2 (mol/kg) = 4.976e-04
Temperature (°C) = 40.00
Electrical balance (eq) = 5.063e-03
Percent error, $100 * (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = 0.42
Iterations = 7
Total H = 1.110129e+02
Total O = 5.555170e+01

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

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	9.538e-07	5.731e-07	-6.021	-6.242	-0.221	-
2.18 H+	6.685e-08	5.012e-08	-7.175	-7.300	-0.125	
0.00 H2O	5.551e+01	9.810e-01	1.744	-0.008	0.000	
18.16 C(4)	4.976e-04					
HCO3-	3.351e-04	2.241e-04	-3.475	-3.650	-0.175	
27.67 MgHCO3+	5.894e-05	3.661e-05	-4.230	-4.436	-0.207	
6.16 CaHCO3+	3.926e-05	2.691e-05	-4.406	-4.570	-0.164	
10.44						

NaHCO3	3.123e-05	3.654e-05	-4.505	-4.437	0.068	
1.80						
CO2	1.940e-05	2.270e-05	-4.712	-4.644	0.068	
35.16						
CaCO3	4.427e-06	5.180e-06	-5.354	-5.286	0.068	-
14.56						
NaCO3-	4.354e-06	3.229e-06	-5.361	-5.491	-0.130	
4.14						
MgCO3	3.522e-06	4.122e-06	-5.453	-5.385	0.068	-
17.10						
CO3-2	1.343e-06	2.683e-07	-5.872	-6.571	-0.699	-
1.64						
(CO2) 2	1.274e-11	1.491e-11	-10.895	-10.827	0.068	
70.32						
Ca	3.426e-02					
Ca+2	3.311e-02	7.959e-03	-1.480	-2.099	-0.619	-
16.45						
CaSO4	1.108e-03	1.296e-03	-2.955	-2.887	0.068	
7.96						
CaHCO3+	3.926e-05	2.691e-05	-4.406	-4.570	-0.164	
10.44						
CaCO3	4.427e-06	5.180e-06	-5.354	-5.286	0.068	-
14.56						
CaOH+	3.486e-08	2.585e-08	-7.458	-7.587	-0.130	
(0)						
CaHSO4+	7.312e-10	5.423e-10	-9.136	-9.266	-0.130	
(0)						
Cl	5.840e-01					
Cl-	5.840e-01	3.637e-01	-0.234	-0.439	-0.206	
19.08						
H(0)	2.637e-26					
H2	1.318e-26	1.543e-26	-25.880	-25.812	0.068	
28.59						
Mg	4.902e-02					
Mg+2	4.591e-02	1.278e-02	-1.338	-1.893	-0.555	-
20.81						
MgSO4	3.045e-03	3.563e-03	-2.516	-2.448	0.068	
6.30						
MgHCO3+	5.894e-05	3.661e-05	-4.230	-4.436	-0.207	
6.16						
MgOH+	4.724e-06	3.299e-06	-5.326	-5.482	-0.156	
(0)						
MgCO3	3.522e-06	4.122e-06	-5.453	-5.385	0.068	-
17.10						
Na	4.450e-01					
Na+	4.428e-01	3.144e-01	-0.354	-0.502	-0.149	
0.05						
NaSO4-	2.124e-03	1.420e-03	-2.673	-2.848	-0.175	
20.94						
NaHCO3	3.123e-05	3.654e-05	-4.505	-4.437	0.068	
1.80						
NaCO3-	4.354e-06	3.229e-06	-5.361	-5.491	-0.130	
4.14						
NaOH	1.540e-17	1.802e-17	-16.812	-16.744	0.068	
(0)						
O(0)	1.171e-36					

O2	5.856e-37	6.852e-37	-36.232	-36.164	0.068
31.40					
S(6)	1.100e-02				
SO4-2	4.724e-03	8.229e-04	-2.326	-3.085	-0.759
19.22					
MgSO4	3.045e-03	3.563e-03	-2.516	-2.448	0.068
6.30					
NaSO4-	2.124e-03	1.420e-03	-2.673	-2.848	-0.175
20.94					
CaSO4	1.108e-03	1.296e-03	-2.955	-2.887	0.068
7.96					
HSO4-	7.642e-09	5.667e-09	-8.117	-8.247	-0.130
41.79					
CaHSO4+	7.312e-10	5.423e-10	-9.136	-9.266	-0.130
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)	
Anhydrite	-0.73	-5.18	-4.45	CaSO4	
Aragonite	-0.22	-8.67	-8.45	CaCO3	
Calcite	-0.09	-8.67	-8.58	CaCO3	
CO2(g)	-3.02	-4.64	-1.63	CO2 Pressure	0.0 atm, phi
1.000					
Dolomite	0.29	-17.14	-17.42	CaMg(CO3)2	
Gypsum	-0.60	-5.20	-4.60	CaSO4:2H2O	
H2(g)	-22.68	-25.81	-3.13	H2	
H2O(g)	-1.15	-0.01	1.14	H2O	
Halite	-2.52	-0.94	1.58	NaCl	
O2(g)	-33.18	-36.16	-2.98	O2	

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using gas phase 1.

-----Fixed-pressure gas phase 1 dissolved completely-----
--

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

Elements	Molality	Moles
C	8.594e-04	8.594e-04
Ca	3.426e-02	3.426e-02
Cl	5.840e-01	5.840e-01
Mg	4.902e-02	4.902e-02

Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	6.059	Charge balance
	pe =	-1.061	Adjusted to redox
equilibrium			
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	68602	
Density (g/cm^3)	=	1.01660	
Volume (L)	=	1.01770	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.822e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	4.975e-04	
Total CO2 (mol/kg)	=	8.594e-04	
Temperature (°C)	=	40.00	
Electrical balance (eq)	=	5.063e-03	
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	0.42	
Iterations	=	12	
Total H	=	1.110129e+02	
Total O	=	5.555242e+01	

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log
			Molality	Activity	Gamma
H+	1.165e-06	8.738e-07	-5.933	-6.059	-0.125
0.00					
OH-	5.471e-08	3.287e-08	-7.262	-7.483	-0.221
2.18					-
H2O	5.551e+01	9.810e-01	1.744	-0.008	0.000
18.16					
C(-4)	1.015e-21				
CH4	1.015e-21	1.188e-21	-20.993	-20.925	0.068
36.62					
C(4)	8.594e-04				
CO2	3.618e-04	4.233e-04	-3.442	-3.373	0.068
35.16					
HCO3-	3.584e-04	2.396e-04	-3.446	-3.620	-0.175
27.67					
MgHCO3+	6.303e-05	3.916e-05	-4.200	-4.407	-0.207
6.16					
CaHCO3+	4.199e-05	2.878e-05	-4.377	-4.541	-0.164
10.44					
NaHCO3	3.340e-05	3.908e-05	-4.476	-4.408	0.068
1.80					
CaCO3	2.715e-07	3.177e-07	-6.566	-6.498	0.068
14.56					-
NaCO3-	2.671e-07	1.981e-07	-6.573	-6.703	-0.130
4.14					

MgCO3	2.161e-07	2.528e-07	-6.665	-6.597	0.068	-
17.10						
CO3-2	8.237e-08	1.646e-08	-7.084	-7.784	-0.699	-
1.64						
(CO2)2	4.428e-09	5.181e-09	-8.354	-8.286	0.068	
70.32						
Ca	3.426e-02					
Ca+2	3.311e-02	7.960e-03	-1.480	-2.099	-0.619	-
16.45						
CaSO4	1.108e-03	1.296e-03	-2.955	-2.887	0.068	
7.96						
CaHCO3+	4.199e-05	2.878e-05	-4.377	-4.541	-0.164	
10.44						
CaCO3	2.715e-07	3.177e-07	-6.566	-6.498	0.068	-
14.56						
CaHSO4+	1.275e-08	9.455e-09	-7.895	-8.024	-0.130	
(0)						
CaOH+	2.000e-09	1.483e-09	-8.699	-8.829	-0.130	
(0)						
Cl	5.840e-01					
Cl-	5.840e-01	3.637e-01	-0.234	-0.439	-0.206	
19.08						
H(0)	1.063e-13					
H2	5.317e-14	6.222e-14	-13.274	-13.206	0.068	
28.59						
Mg	4.902e-02					
Mg+2	4.591e-02	1.278e-02	-1.338	-1.893	-0.555	-
20.81						
MgSO4	3.045e-03	3.563e-03	-2.516	-2.448	0.068	
6.30						
MgHCO3+	6.303e-05	3.916e-05	-4.200	-4.407	-0.207	
6.16						
MgOH+	2.710e-07	1.892e-07	-6.567	-6.723	-0.156	
(0)						
MgCO3	2.161e-07	2.528e-07	-6.665	-6.597	0.068	-
17.10						
Na	4.450e-01					
Na+	4.428e-01	3.144e-01	-0.354	-0.502	-0.149	
0.05						
NaSO4-	2.123e-03	1.420e-03	-2.673	-2.848	-0.175	
20.94						
NaHCO3	3.340e-05	3.908e-05	-4.476	-4.408	0.068	
1.80						
NaCO3-	2.671e-07	1.981e-07	-6.573	-6.703	-0.130	
4.14						
NaOH	8.834e-19	1.034e-18	-18.054	-17.986	0.068	
(0)						
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-61.444	-61.375	0.068	
31.40						
S(-2)	1.721e-17					
H2S	1.251e-17	1.463e-17	-16.903	-16.835	0.068	
37.21						
HS-	4.703e-18	2.826e-18	-17.328	-17.549	-0.221	
21.91						
S-2	5.601e-24	1.039e-24	-23.252	-23.983	-0.732	
(0)						

S (6)	1.100e-02					
SO4-2	4.724e-03	8.229e-04	-2.326	-3.085	-0.759	
19.22						
MgSO4	3.045e-03	3.563e-03	-2.516	-2.448	0.068	
6.30						
NaSO4-	2.123e-03	1.420e-03	-2.673	-2.848	-0.175	
20.94						
CaSO4	1.108e-03	1.296e-03	-2.955	-2.887	0.068	
7.96						
HSO4-	1.332e-07	9.880e-08	-6.875	-7.005	-0.130	
41.79						
CaHSO4+	1.275e-08	9.455e-09	-7.895	-8.024	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.73	-5.18	-4.45	CaSO4
Aragonite	-1.44	-9.88	-8.45	CaCO3
Calcite	-1.30	-9.88	-8.58	CaCO3
CH4 (g)	-18.01	-20.93	-2.91	CH4
CO2 (g)	-1.75	-3.37	-1.63	CO2
Dolomite	-2.14	-19.56	-17.42	CaMg (CO3) 2
Gypsum	-0.60	-5.20	-4.60	CaSO4:2H2O
H2 (g)	-10.08	-13.21	-3.13	H2
H2O (g)	-1.15	-0.01	1.14	H2O
H2S (g)	-15.65	-23.61	-7.96	H2S
Halite	-2.52	-0.94	1.58	NaCl
O2 (g)	-58.39	-61.38	-2.98	O2
Sulfur	-11.39	-6.84	4.55	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

 Reading input data for simulation 2.

 End of Run after 0.36 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
 1\Appendix\SP\sp_ID=0.5.pqi
 Output file: D:\KU\Thesis Writing\4) Results\Story
 1\Appendix\SP\sp_ID=0.5.pqo
 Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
 15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 36
Mg 55.13
Na 509
S(6) 12.6
Alkalinity 0.8 as HCO3-
Cl 653
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	8.000e-04	8.000e-04
Ca	3.600e-02	3.600e-02
Cl	6.530e-01	6.530e-01
Mg	5.513e-02	5.513e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

pH = 8.200
pe = 4.000

Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C) = 75601
 Density (g/cm^3) = 1.01956
 Volume (L) = 1.01895
 Activity of water = 0.979
 Ionic strength (mol/kgw) = $7.641\text{e-}01$
 Mass of water (kg) = $1.000\text{e+}00$
 Total carbon (mol/kg) = $6.297\text{e-}04$
 Total CO_2 (mol/kg) = $6.297\text{e-}04$
 Temperature ($^\circ\text{C}$) = 40.00
 Electrical balance (eq) = $1.226\text{e-}02$
 Percent error, $100 * (\text{Cat-}|\text{An}|) / (\text{Cat+}|\text{An}|)$ = 0.91
 Iterations = 6
 Total H = $1.110130\text{e+}02$
 Total O = $5.555855\text{e+}01$

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

--

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm^3/mol						
OH-	$7.670\text{e-}06$	$4.541\text{e-}06$	-5.115	-5.343	-0.228	-
2.04						
H+	$8.455\text{e-}09$	$6.310\text{e-}09$	-8.073	-8.200	-0.127	
0.00						
H ₂ O	$5.551\text{e+}01$	$9.786\text{e-}01$	1.744	-0.009	0.000	
18.16						
C(4)	$6.297\text{e-}04$					
HCO ₃ -	$3.545\text{e-}04$	$2.349\text{e-}04$	-3.450	-3.629	-0.179	
27.89						
MgHCO ₃ +	$7.024\text{e-}05$	$4.307\text{e-}05$	-4.153	-4.366	-0.212	
6.17						
CaHCO ₃ +	$4.311\text{e-}05$	$2.932\text{e-}05$	-4.365	-4.533	-0.167	
10.45						
NaCO ₃ -	$4.104\text{e-}05$	$3.082\text{e-}05$	-4.387	-4.511	-0.124	
4.61						
CaCO ₃	$3.759\text{e-}05$	$4.482\text{e-}05$	-4.425	-4.349	0.076	-
14.56						
NaHCO ₃	$3.683\text{e-}05$	$4.392\text{e-}05$	-4.434	-4.357	0.076	
1.80						
MgCO ₃	$3.230\text{e-}05$	$3.851\text{e-}05$	-4.491	-4.414	0.076	-
17.10						
CO ₃ -2	$1.160\text{e-}05$	$2.234\text{e-}06$	-4.936	-5.651	-0.715	-
1.46						
CO ₂	$2.519\text{e-}06$	$3.003\text{e-}06$	-5.599	-5.522	0.076	
35.16						
(CO ₂) ₂	$2.187\text{e-}13$	$2.608\text{e-}13$	-12.660	-12.584	0.076	
70.32						
Ca	$3.600\text{e-}02$					
Ca+2	$3.472\text{e-}02$	$8.272\text{e-}03$	-1.459	-2.082	-0.623	-
16.38						
CaSO ₄	$1.197\text{e-}03$	$1.427\text{e-}03$	-2.922	-2.846	0.076	
7.96						
CaHCO ₃ +	$4.311\text{e-}05$	$2.932\text{e-}05$	-4.365	-4.533	-0.167	
10.45						

CaCO3	3.759e-05	4.482e-05	-4.425	-4.349	0.076	-
14.56						
CaOH+	2.835e-07	2.129e-07	-6.547	-6.672	-0.124	
(0)						
CaHSO4+	1.001e-10	7.516e-11	-10.000	-10.124	-0.124	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.022e-01	-0.185	-0.396	-0.210	
19.13						
H(0)	4.101e-28					
H2	2.050e-28	2.445e-28	-27.688	-27.612	0.076	
28.59						
Mg	5.513e-02					
Mg+2	5.143e-02	1.435e-02	-1.289	-1.843	-0.554	-
20.74						
MgSO4	3.552e-03	4.236e-03	-2.449	-2.373	0.076	
6.30						
MgHCO3+	7.024e-05	4.307e-05	-4.153	-4.366	-0.212	
6.17						
MgOH+	4.232e-05	2.934e-05	-4.373	-4.533	-0.159	
(0)						
MgCO3	3.230e-05	3.851e-05	-4.491	-4.414	0.076	-
17.10						
Na	5.090e-01					
Na+	5.063e-01	3.605e-01	-0.296	-0.443	-0.147	
0.10						
NaSO4-	2.603e-03	1.724e-03	-2.585	-2.763	-0.179	
21.45						
NaCO3-	4.104e-05	3.082e-05	-4.387	-4.511	-0.124	
4.61						
NaHCO3	3.683e-05	4.392e-05	-4.434	-4.357	0.076	
1.80						
NaOH	1.373e-16	1.637e-16	-15.862	-15.786	0.076	
(0)						
O(0)	4.553e-33					
O2	2.277e-33	2.715e-33	-32.643	-32.566	0.076	
31.40						
S(6)	1.260e-02					
SO4-2	5.248e-03	8.717e-04	-2.280	-3.060	-0.780	
19.43						
MgSO4	3.552e-03	4.236e-03	-2.449	-2.373	0.076	
6.30						
NaSO4-	2.603e-03	1.724e-03	-2.585	-2.763	-0.179	
21.45						
CaSO4	1.197e-03	1.427e-03	-2.922	-2.846	0.076	
7.96						
HSO4-	1.006e-09	7.557e-10	-8.997	-9.122	-0.124	
41.83						
CaHSO4+	1.001e-10	7.516e-11	-10.000	-10.124	-0.124	
(0)						

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

Phase	SI**	log IAP	log K(313 K, 1 atm)
Anhydrite	-0.69	-5.14	-4.45 CaSO4

Aragonite	0.71	-7.73	-8.45	CaCO3
Calcite	0.85	-7.73	-8.58	CaCO3
CO2(g)	-3.90	-5.52	-1.63	CO2
Dolomite	2.19	-15.23	-17.42	CaMg(CO3)2
Gypsum	-0.56	-5.16	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-29.58	-32.57	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.132 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=1.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=1.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat
SOLUTION 1
temp 40
pH 7.62
pe 4
redox pe

```

units      mmol/kgw
density    1
Ca         36.0
Mg         55.0
Na         509
S(6)      12.6
Alkalinity 0.71 as HCO3-
Cl         653
water     1 # kgg

```

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	7.100e-04	7.100e-04
Ca	3.600e-02	3.600e-02
Cl	6.530e-01	6.530e-01
Mg	5.500e-02	5.500e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

```

pH = 7.620
pe = 4.000
Specific Conductance (µS/cm, 40°C) = 75598
Density (g/cm³) = 1.01955
Volume (L) = 1.01896
Activity of water = 0.979
Ionic strength (mol/kgw) = 7.639e-01
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 6.691e-04
Total CO2 (mol/kg) = 6.691e-04
Temperature (°C) = 40.00
Electrical balance (eq) = 1.209e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.90
Iterations = 7
Total H = 1.110131e+02
Total O = 5.555863e+01

```

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

mole V Species cm³/mol	Molality	Activity	Log	Log	Log	Gamma
			Molality	Activity	Gamma	
OH- 2.04	2.017e-06	1.194e-06	-5.695	-5.923	-0.228	-

H+	3.215e-08	2.399e-08	-7.493	-7.620	-0.127	
0.00						
H2O	5.551e+01	9.786e-01	1.744	-0.009	0.000	
18.16						
C(4)	6.691e-04					
HCO3-	4.341e-04	2.876e-04	-3.362	-3.541	-0.179	
27.89						
MgHCO3+	8.587e-05	5.266e-05	-4.066	-4.279	-0.212	
6.17						
CaHCO3+	5.282e-05	3.592e-05	-4.277	-4.445	-0.167	
10.45						
NaHCO3	4.511e-05	5.379e-05	-4.346	-4.269	0.076	
1.80						
NaCO3-	1.322e-05	9.929e-06	-4.879	-5.003	-0.124	
4.61						
CaCO3	1.211e-05	1.444e-05	-4.917	-4.840	0.076	-
14.56						
CO2	1.173e-05	1.398e-05	-4.931	-4.854	0.076	
35.16						
MgCO3	1.039e-05	1.238e-05	-4.984	-4.907	0.076	-
17.10						
CO3-2	3.735e-06	7.196e-07	-5.428	-6.143	-0.715	-
1.46						
(CO2)2	4.741e-12	5.653e-12	-11.324	-11.248	0.076	
70.32						
Ca	3.600e-02					
Ca+2	3.474e-02	8.276e-03	-1.459	-2.082	-0.623	-
16.38						
CaSO4	1.198e-03	1.429e-03	-2.922	-2.845	0.076	
7.96						
CaHCO3+	5.282e-05	3.592e-05	-4.277	-4.445	-0.167	
10.45						
CaCO3	1.211e-05	1.444e-05	-4.917	-4.840	0.076	-
14.56						
CaOH+	7.460e-08	5.603e-08	-7.127	-7.252	-0.124	
(0)						
CaHSO4+	3.808e-10	2.860e-10	-9.419	-9.544	-0.124	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.022e-01	-0.185	-0.396	-0.210	
19.13						
H(0)	5.928e-27					
H2	2.964e-27	3.534e-27	-26.528	-26.452	0.076	
28.59						
Mg	5.500e-02					
Mg+2	5.134e-02	1.432e-02	-1.290	-1.844	-0.554	-
20.74						
MgSO4	3.548e-03	4.230e-03	-2.450	-2.374	0.076	
6.30						
MgHCO3+	8.587e-05	5.266e-05	-4.066	-4.279	-0.212	
6.17						
MgOH+	1.111e-05	7.704e-06	-4.954	-5.113	-0.159	
(0)						
MgCO3	1.039e-05	1.238e-05	-4.984	-4.907	0.076	-
17.10						
Na	5.090e-01					

Na+	5.063e-01	3.606e-01	-0.296	-0.443	-0.147
0.10					
NaSO4-	2.604e-03	1.725e-03	-2.584	-2.763	-0.179
21.44					
NaHCO3	4.511e-05	5.379e-05	-4.346	-4.269	0.076
1.80					
NaCO3-	1.322e-05	9.929e-06	-4.879	-5.003	-0.124
4.61					
NaOH	3.612e-17	4.307e-17	-16.442	-16.366	0.076
(0)					
O(0)	2.179e-35				
O2	1.090e-35	1.299e-35	-34.963	-34.886	0.076
31.40					
S(6)	1.260e-02				
SO4-2	5.250e-03	8.721e-04	-2.280	-3.059	-0.780
19.43					
MgSO4	3.548e-03	4.230e-03	-2.450	-2.374	0.076
6.30					
NaSO4-	2.604e-03	1.725e-03	-2.584	-2.763	-0.179
21.44					
CaSO4	1.198e-03	1.429e-03	-2.922	-2.845	0.076
7.96					
HSO4-	3.827e-09	2.874e-09	-8.417	-8.541	-0.124
41.83					
CaHSO4+	3.808e-10	2.860e-10	-9.419	-9.544	-0.124
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.69	-5.14	-4.45	CaSO4
Aragonite	0.22	-8.23	-8.45	CaCO3
Calcite	0.35	-8.23	-8.58	CaCO3
CO2(g)	-3.23	-4.85	-1.63	CO2
Dolomite	1.21	-16.21	-17.42	CaMg(CO3)2
Gypsum	-0.56	-5.16	-4.60	CaSO4:2H2O
H2(g)	-23.32	-26.45	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-31.90	-34.89	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

 Reading input data for simulation 2.

 End of Run after 0.133 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=2.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=2.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.63
pe 4
redox pe
units mmol/kgw
density 1
Ca 37.02
Mg 56.58
Na 509
S(6) 12.6
Alkalinity 0.71 as HCO3-
Cl 653
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	7.100e-04	7.100e-04
Ca	3.702e-02	3.702e-02
Cl	6.530e-01	6.530e-01
Mg	5.658e-02	5.658e-02

Na 5.090e-01 5.090e-01
 S(6) 1.260e-02 1.260e-02

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

pH = 7.630
 pe = 4.000
 Specific Conductance (µS/cm, 40°C) = 75702
 Density (g/cm³) = 1.01968
 Volume (L) = 1.01891
 Activity of water = 0.979
 Ionic strength (mol/kgw) = 7.689e-01
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 6.669e-04
 Total CO2 (mol/kg) = 6.669e-04
 Temperature (°C) = 40.00
 Electrical balance (eq) = 1.729e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.28
 Iterations = 7
 Total H = 1.110131e+02
 Total O = 5.555862e+01

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

mole V Species cm³/mol	Molality	Activity	Log		Gamma	
			Molality	Activity		
OH-	2.066e-06	1.222e-06	-5.685	-5.913	-0.228	-
2.03						
H+	3.142e-08	2.344e-08	-7.503	-7.630	-0.127	
0.00						
H2O	5.551e+01	9.786e-01	1.744	-0.009	0.000	
18.16						
C(4)	6.669e-04					
HCO3-	4.293e-04	2.843e-04	-3.367	-3.546	-0.179	
27.90						
MgHCO3+	8.747e-05	5.360e-05	-4.058	-4.271	-0.213	
6.17						
CaHCO3+	5.372e-05	3.651e-05	-4.270	-4.438	-0.168	
10.45						
NaHCO3	4.455e-05	5.318e-05	-4.351	-4.274	0.077	
1.80						
NaCO3-	1.337e-05	1.005e-05	-4.874	-4.998	-0.124	
4.64						
CaCO3	1.259e-05	1.502e-05	-4.900	-4.823	0.077	-
14.56						
CO2	1.132e-05	1.351e-05	-4.946	-4.869	0.077	
35.16						
MgCO3	1.081e-05	1.290e-05	-4.966	-4.889	0.077	-
17.10						
CO3-2	3.786e-06	7.279e-07	-5.422	-6.138	-0.716	-
1.45						

(CO2)2	4.420e-12	5.276e-12	-11.355	-11.278	0.077	
70.32						
Ca	3.702e-02					
Ca+2	3.574e-02	8.511e-03	-1.447	-2.070	-0.623	-
16.38						
CaSO4	1.216e-03	1.452e-03	-2.915	-2.838	0.077	
7.96						
CaHCO3+	5.372e-05	3.651e-05	-4.270	-4.438	-0.168	
10.45						
CaCO3	1.259e-05	1.502e-05	-4.900	-4.823	0.077	-
14.56						
CaOH+	7.844e-08	5.896e-08	-7.105	-7.229	-0.124	
(0)						
CaHSO4+	3.779e-10	2.840e-10	-9.423	-9.547	-0.124	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.020e-01	-0.185	-0.396	-0.211	
19.13						
H(0)	5.654e-27					
H2	2.827e-27	3.375e-27	-26.549	-26.472	0.077	
28.59						
Mg	5.658e-02					
Mg+2	5.286e-02	1.475e-02	-1.277	-1.831	-0.554	-
20.74						
MgSO4	3.606e-03	4.305e-03	-2.443	-2.366	0.077	
6.30						
MgHCO3+	8.747e-05	5.360e-05	-4.058	-4.271	-0.213	
6.17						
MgOH+	1.171e-05	8.119e-06	-4.931	-5.091	-0.159	
(0)						
MgCO3	1.081e-05	1.290e-05	-4.966	-4.889	0.077	-
17.10						
Na	5.090e-01					
Na+	5.064e-01	3.607e-01	-0.296	-0.443	-0.147	
0.10						
NaSO4-	2.575e-03	1.705e-03	-2.589	-2.768	-0.179	
21.47						
NaHCO3	4.455e-05	5.318e-05	-4.351	-4.274	0.077	
1.80						
NaCO3-	1.337e-05	1.005e-05	-4.874	-4.998	-0.124	
4.64						
NaOH	3.693e-17	4.408e-17	-16.433	-16.356	0.077	
(0)						
O(0)	2.387e-35					
O2	1.193e-35	1.425e-35	-34.923	-34.846	0.077	
31.40						
S(6)	1.260e-02					
SO4-2	5.202e-03	8.618e-04	-2.284	-3.065	-0.781	
19.45						
MgSO4	3.606e-03	4.305e-03	-2.443	-2.366	0.077	
6.30						
NaSO4-	2.575e-03	1.705e-03	-2.589	-2.768	-0.179	
21.47						
CaSO4	1.216e-03	1.452e-03	-2.915	-2.838	0.077	
7.96						
HSO4-	3.693e-09	2.776e-09	-8.433	-8.557	-0.124	
41.83						

CaHSO4+ 3.779e-10 2.840e-10 -9.423 -9.547 -0.124
(0)

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.68	-5.13	-4.45	CaSO4
Aragonite	0.24	-8.21	-8.45	CaCO3
Calcite	0.37	-8.21	-8.58	CaCO3
CO2(g)	-3.24	-4.87	-1.63	CO2
Dolomite	1.24	-16.18	-17.42	CaMg(CO3)2
Gypsum	-0.56	-5.15	-4.60	CaSO4:2H2O
H2(g)	-23.34	-26.47	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-31.86	-34.85	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.131 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=5.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=5.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.72
pe 4
redox pe
units mmol/kgw
density 1
Ca 37.76
Mg 57.73
Na 509
S(6) 12.6
Alkalinity 0.675 as HCO3-
Cl 653
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	6.750e-04	6.750e-04
Ca	3.776e-02	3.776e-02
Cl	6.530e-01	6.530e-01
Mg	5.773e-02	5.773e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

pH	=	7.720
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	75777
Density (g/cm^3)	=	1.01977
Volume (L)	=	1.01888
Activity of water	=	0.979
Ionic strength (mol/kgw)	=	7.725e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	6.199e-04
Total CO2 (mol/kg)	=	6.199e-04
Temperature (°C)	=	40.00
Electrical balance (eq)	=	2.111e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.56
Iterations	=	7
Total H	=	1.110130e+02
Total O	=	5.555849e+01

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

--

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	2.543e-06	1.504e-06	-5.595	-5.823	-0.228	-
2.03						
H+	2.555e-08	1.905e-08	-7.593	-7.720	-0.127	
0.00						
H2O	5.551e+01	9.785e-01	1.744	-0.009	0.000	
18.16						
C(4)	6.199e-04					
HCO3-	3.928e-04	2.600e-04	-3.406	-3.585	-0.179	
27.91						
MgHCO3+	8.174e-05	5.006e-05	-4.088	-4.301	-0.213	
6.17						
CaHCO3+	5.013e-05	3.407e-05	-4.300	-4.468	-0.168	
10.45						
NaHCO3	4.072e-05	4.865e-05	-4.390	-4.313	0.077	
1.80						
NaCO3-	1.503e-05	1.131e-05	-4.823	-4.947	-0.124	
4.66						
CaCO3	1.443e-05	1.724e-05	-4.841	-4.763	0.077	-
14.56						
MgCO3	1.241e-05	1.482e-05	-4.906	-4.829	0.077	-
17.10						
CO2	8.405e-06	1.004e-05	-5.075	-4.998	0.077	
35.16						
CO3-2	4.266e-06	8.190e-07	-5.370	-6.087	-0.717	-
1.44						
(CO2)2	2.440e-12	2.915e-12	-11.613	-11.535	0.077	
70.32						
Ca	3.776e-02					
Ca+2	3.647e-02	8.682e-03	-1.438	-2.061	-0.623	-
16.38						
CaSO4	1.229e-03	1.468e-03	-2.910	-2.833	0.077	
7.96						
CaHCO3+	5.013e-05	3.407e-05	-4.300	-4.468	-0.168	
10.45						
CaCO3	1.443e-05	1.724e-05	-4.841	-4.763	0.077	-
14.56						
CaOH+	9.838e-08	7.399e-08	-7.007	-7.131	-0.124	
(0)						
CaHSO4+	3.105e-10	2.335e-10	-9.508	-9.632	-0.124	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.018e-01	-0.185	-0.396	-0.211	
19.13						
H(0)	3.733e-27					
H2	1.866e-27	2.230e-27	-26.729	-26.652	0.077	
28.59						
Mg	5.773e-02					
Mg+2	5.397e-02	1.506e-02	-1.268	-1.822	-0.554	-
20.73						

MgSO4	3.648e-03	4.359e-03	-2.438	-2.361	0.077	
6.30						
MgHCO3+	8.174e-05	5.006e-05	-4.088	-4.301	-0.213	
6.17						
MgOH+	1.472e-05	1.020e-05	-4.832	-4.991	-0.159	
(0)						
MgCO3	1.241e-05	1.482e-05	-4.906	-4.829	0.077	-
17.10						
Na	5.090e-01					
Na+	5.064e-01	3.607e-01	-0.296	-0.443	-0.147	
0.10						
NaSO4-	2.555e-03	1.691e-03	-2.593	-2.772	-0.179	
21.49						
NaHCO3	4.072e-05	4.865e-05	-4.390	-4.313	0.077	
1.80						
NaCO3-	1.503e-05	1.131e-05	-4.823	-4.947	-0.124	
4.66						
NaOH	4.540e-17	5.424e-17	-16.343	-16.266	0.077	
(0)						
O(0)	5.463e-35					
O2	2.732e-35	3.263e-35	-34.564	-34.486	0.077	
31.40						
S(6)	1.260e-02					
SO4-2	5.168e-03	8.544e-04	-2.287	-3.068	-0.782	
19.45						
MgSO4	3.648e-03	4.359e-03	-2.438	-2.361	0.077	
6.30						
NaSO4-	2.555e-03	1.691e-03	-2.593	-2.772	-0.179	
21.49						
CaSO4	1.229e-03	1.468e-03	-2.910	-2.833	0.077	
7.96						
HSO4-	2.974e-09	2.237e-09	-8.527	-8.650	-0.124	
41.83						
CaHSO4+	3.105e-10	2.335e-10	-9.508	-9.632	-0.124	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.68	-5.13	-4.45	CaSO4
Aragonite	0.30	-8.15	-8.45	CaCO3
Calcite	0.43	-8.15	-8.58	CaCO3
CO2(g)	-3.37	-5.00	-1.63	CO2
Dolomite	1.36	-16.06	-17.42	CaMg(CO3)2
Gypsum	-0.55	-5.15	-4.60	CaSO4:2H2O
H2(g)	-23.52	-26.65	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-31.50	-34.49	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

Reading input data for simulation 2.

End of Run after 0.13 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=10.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=10.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat
SOLUTION 1
temp 40
pH 7.75
pe 4
redox pe
units mmol/kgw
density 1
Ca 40.23
Mg 61.24
Na 509
S(6) 12.6
Alkalinity 0.685 as HCO3-
Cl 653
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

--

Elements	Molality	Moles
Alkalinity	6.850e-04	6.850e-04
Ca	4.023e-02	4.023e-02
Cl	6.530e-01	6.530e-01
Mg	6.124e-02	6.124e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

--

pH	=	7.750
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	76018
Density (g/cm^3)	=	1.02005
Volume (L)	=	1.01878
Activity of water	=	0.978
Ionic strength (mol/kgw)	=	7.839e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	6.227e-04
Total CO2 (mol/kg)	=	6.227e-04
Temperature (°C)	=	40.00
Electrical balance (eq)	=	3.306e-02
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	2.42
Iterations	=	7
Total H	=	1.110130e+02
Total O	=	5.555850e+01

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	2.730e-06	1.611e-06	-5.564	-5.793	-0.229	-
2.01						
H+	2.386e-08	1.778e-08	-7.622	-7.750	-0.128	
0.00						
H2O	5.551e+01	9.784e-01	1.744	-0.009	0.000	
18.16						
C(4)	6.227e-04					
HCO3-	3.866e-04	2.556e-04	-3.413	-3.592	-0.180	
27.94						
MgHCO3+	8.558e-05	5.233e-05	-4.068	-4.281	-0.214	
6.17						
CaHCO3+	5.257e-05	3.568e-05	-4.279	-4.448	-0.168	
10.45						
NaHCO3	3.995e-05	4.785e-05	-4.398	-4.320	0.078	
1.80						
CaCO3	1.616e-05	1.935e-05	-4.792	-4.713	0.078	-
14.56						

NaCO3-	1.581e-05	1.192e-05	-4.801	-4.924	-0.123	
4.72						
MgCO3	1.386e-05	1.660e-05	-4.858	-4.780	0.078	-
17.10						
CO2	7.692e-06	9.214e-06	-5.114	-5.036	0.078	
35.16						
CO3-2	4.515e-06	8.627e-07	-5.345	-6.064	-0.719	-
1.41						
(CO2) 2	2.049e-12	2.454e-12	-11.688	-11.610	0.078	
70.32						
Ca	4.023e-02					
Ca+2	3.889e-02	9.251e-03	-1.410	-2.034	-0.624	-
16.37						
CaSO4	1.272e-03	1.524e-03	-2.895	-2.817	0.078	
7.96						
CaHCO3+	5.257e-05	3.568e-05	-4.279	-4.448	-0.168	
10.45						
CaCO3	1.616e-05	1.935e-05	-4.792	-4.713	0.078	-
14.56						
CaOH+	1.121e-07	8.447e-08	-6.950	-7.073	-0.123	
(0)						
CaHSO4+	3.001e-10	2.262e-10	-9.523	-9.646	-0.123	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.012e-01	-0.185	-0.397	-0.212	
19.14						
H(0)	3.243e-27					
H2	1.621e-27	1.942e-27	-26.790	-26.712	0.078	
28.59						
Mg	6.124e-02					
Mg+2	5.735e-02	1.602e-02	-1.241	-1.795	-0.554	-
20.72						
MgSO4	3.769e-03	4.515e-03	-2.424	-2.345	0.078	
6.30						
MgHCO3+	8.558e-05	5.233e-05	-4.068	-4.281	-0.214	
6.17						
MgOH+	1.679e-05	1.162e-05	-4.775	-4.935	-0.160	
(0)						
MgCO3	1.386e-05	1.660e-05	-4.858	-4.780	0.078	-
17.10						
Na	5.090e-01					
Na+	5.065e-01	3.610e-01	-0.295	-0.443	-0.147	
0.11						
NaSO4-	2.493e-03	1.648e-03	-2.603	-2.783	-0.180	
21.56						
NaHCO3	3.995e-05	4.785e-05	-4.398	-4.320	0.078	
1.80						
NaCO3-	1.581e-05	1.192e-05	-4.801	-4.924	-0.123	
4.72						
NaOH	4.855e-17	5.815e-17	-16.314	-16.235	0.078	
(0)						
O(0)	7.181e-35					
O2	3.591e-35	4.301e-35	-34.445	-34.366	0.078	
31.40						
S(6)	1.260e-02					
SO4-2	5.065e-03	8.323e-04	-2.295	-3.080	-0.784	
19.48						

MgSO4	3.769e-03	4.515e-03	-2.424	-2.345	0.078
6.30					
NaSO4-	2.493e-03	1.648e-03	-2.603	-2.783	-0.180
21.56					
CaSO4	1.272e-03	1.524e-03	-2.895	-2.817	0.078
7.96					
HSO4-	2.699e-09	2.034e-09	-8.569	-8.692	-0.123
41.84					
CaHSO4+	3.001e-10	2.262e-10	-9.523	-9.646	-0.123
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.66	-5.11	-4.45	CaSO4
Aragonite	0.35	-8.10	-8.45	CaCO3
Calcite	0.48	-8.10	-8.58	CaCO3
CO2 (g)	-3.41	-5.04	-1.63	CO2
Dolomite	1.46	-15.96	-17.42	CaMg(CO3)2
Gypsum	-0.54	-5.13	-4.60	CaSO4:2H2O
H2 (g)	-23.58	-26.71	-3.13	H2
H2O (g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2 (g)	-31.38	-34.37	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.158 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=15.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=15.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.63
pe 4
redox pe
units mmol/kgw
density 1
Ca 39.97
Mg 60.98
Na 509
S(6) 12.6
Alkalinity 0.72 as HCO3-
Cl 653
water 1 # kgw

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	7.200e-04	7.200e-04
Ca	3.997e-02	3.997e-02
Cl	6.530e-01	6.530e-01
Mg	6.098e-02	6.098e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

pH	=	7.630
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	75997
Density (g/cm^3)	=	1.02003
Volume (L)	=	1.01879
Activity of water	=	0.978
Ionic strength (mol/kgw)	=	7.829e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	6.744e-04
Total CO2 (mol/kg)	=	6.744e-04

Temperature (°C) = 40.00
 Electrical balance (eq) = 3.198e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 2.34
 Iterations = 7
 Total H = 1.110131e+02
 Total O = 5.555864e+01

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

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	2.071e-06	1.222e-06	-5.684	-5.913	-0.229	-
2.01						
H+	3.145e-08	2.344e-08	-7.502	-7.630	-0.128	
0.00						
H2O	5.551e+01	9.784e-01	1.744	-0.009	0.000	
18.16						
C(4)	6.744e-04					
HCO3-	4.259e-04	2.816e-04	-3.371	-3.550	-0.180	
27.94						
MgHCO3+	9.386e-05	5.740e-05	-4.028	-4.241	-0.214	
6.17						
CaHCO3+	5.753e-05	3.906e-05	-4.240	-4.408	-0.168	
10.45						
NaHCO3	4.402e-05	5.272e-05	-4.356	-4.278	0.078	
1.80						
CaCO3	1.342e-05	1.607e-05	-4.872	-4.794	0.078	-
14.56						
NaCO3-	1.322e-05	9.959e-06	-4.879	-5.002	-0.123	
4.72						
MgCO3	1.154e-05	1.381e-05	-4.938	-4.860	0.078	-
17.10						
CO2	1.117e-05	1.338e-05	-4.952	-4.873	0.078	
35.16						
CO3-2	3.772e-06	7.210e-07	-5.423	-6.142	-0.719	-
1.42						
(CO2)2	4.324e-12	5.178e-12	-11.364	-11.286	0.078	
70.32						
Ca	3.997e-02					
Ca+2	3.863e-02	9.190e-03	-1.413	-2.037	-0.624	-
16.37						
CaSO4	1.267e-03	1.517e-03	-2.897	-2.819	0.078	
7.96						
CaHCO3+	5.753e-05	3.906e-05	-4.240	-4.408	-0.168	
10.45						
CaCO3	1.342e-05	1.607e-05	-4.872	-4.794	0.078	-
14.56						
CaOH+	8.449e-08	6.366e-08	-7.073	-7.196	-0.123	
(0)						
CaHSO4+	3.940e-10	2.969e-10	-9.405	-9.527	-0.123	
(0)						
Cl	6.530e-01					

Cl-	6.530e-01	4.013e-01	-0.185	-0.397	-0.211	
19.14						
H(0)	5.636e-27					
H2	2.818e-27	3.375e-27	-26.550	-26.472	0.078	
28.59						
Mg	6.098e-02					
Mg+2	5.710e-02	1.595e-02	-1.243	-1.797	-0.554	-
20.72						
MgSO4	3.761e-03	4.504e-03	-2.425	-2.346	0.078	
6.30						
MgHCO3+	9.386e-05	5.740e-05	-4.028	-4.241	-0.214	
6.17						
MgOH+	1.268e-05	8.775e-06	-4.897	-5.057	-0.160	
(0)						
MgCO3	1.154e-05	1.381e-05	-4.938	-4.860	0.078	-
17.10						
Na	5.090e-01					
Na+	5.064e-01	3.609e-01	-0.295	-0.443	-0.147	
0.11						
NaSO4-	2.498e-03	1.652e-03	-2.602	-2.782	-0.180	
21.56						
NaHCO3	4.402e-05	5.272e-05	-4.356	-4.278	0.078	
1.80						
NaCO3-	1.322e-05	9.959e-06	-4.879	-5.002	-0.123	
4.72						
NaOH	3.683e-17	4.411e-17	-16.434	-16.355	0.078	
(0)						
O(0)	2.379e-35					
O2	1.189e-35	1.424e-35	-34.925	-34.846	0.078	
31.40						
S(6)	1.260e-02					
SO4-2	5.074e-03	8.341e-04	-2.295	-3.079	-0.784	
19.48						
MgSO4	3.761e-03	4.504e-03	-2.425	-2.346	0.078	
6.30						
NaSO4-	2.498e-03	1.652e-03	-2.602	-2.782	-0.180	
21.56						
CaSO4	1.267e-03	1.517e-03	-2.897	-2.819	0.078	
7.96						
HSO4-	3.566e-09	2.687e-09	-8.448	-8.571	-0.123	
41.84						
CaHSO4+	3.940e-10	2.969e-10	-9.405	-9.527	-0.123	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.66	-5.12	-4.45	CaSO4
Aragonite	0.27	-8.18	-8.45	CaCO3
Calcite	0.40	-8.18	-8.58	CaCO3
CO2(g)	-3.25	-4.87	-1.63	CO2
Dolomite	1.30	-16.12	-17.42	CaMg(CO3)2
Gypsum	-0.54	-5.13	-4.60	CaSO4:2H2O
H2(g)	-23.34	-26.47	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O

Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-31.86	-34.85	-2.98	O2

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.14 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=20.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=20.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.56
pe 4
redox pe
units mmol/kgw
density 1
Ca 38.4
Mg 58.08
Na 509
S(6) 12.6
Alkalinity 0.69 as HCO3-

Cl 653
 water 1 # kgg

 Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	6.900e-04	6.900e-04
Ca	3.840e-02	3.840e-02
Cl	6.530e-01	6.530e-01
Mg	5.808e-02	5.808e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

pH	=	7.560
pe	=	4.000
Specific Conductance (µS/cm, 40°C)	=	75821
Density (g/cm³)	=	1.01982
Volume (L)	=	1.01886
Activity of water	=	0.979
Ionic strength (mol/kgw)	=	7.744e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	6.565e-04
Total CO2 (mol/kg)	=	6.565e-04
Temperature (°C)	=	40.00
Electrical balance (eq)	=	2.307e-02
Percent error, 100*(Cat- An)/(Cat+ An)	=	1.70
Iterations	=	7
Total H	=	1.110131e+02
Total O	=	5.555859e+01

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

mole V Species cm³/mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.760e-06	1.040e-06	-5.754	-5.983	-0.228	-
2.02 H+	3.693e-08	2.754e-08	-7.433	-7.560	-0.127	
0.00 H2O	5.551e+01	9.785e-01	1.744	-0.009	0.000	
18.16 C(4)	6.565e-04					
HCO3-	4.220e-04	2.793e-04	-3.375	-3.554	-0.179	
27.92						

MgHCO3+	8.839e-05	5.412e-05	-4.054	-4.267	-0.213	
6.17						
CaHCO3+	5.477e-05	3.721e-05	-4.261	-4.429	-0.168	
10.45						
NaHCO3	4.373e-05	5.226e-05	-4.359	-4.282	0.077	
1.80						
CO2	1.305e-05	1.559e-05	-4.885	-4.807	0.077	
35.16						
NaCO3-	1.117e-05	8.403e-06	-4.952	-5.076	-0.124	
4.67						
CaCO3	1.090e-05	1.303e-05	-4.962	-4.885	0.077	-
14.56						
MgCO3	9.276e-06	1.109e-05	-5.033	-4.955	0.077	-
17.10						
CO3-2	3.173e-06	6.087e-07	-5.499	-6.216	-0.717	-
1.43						
(CO2) 2	5.881e-12	7.029e-12	-11.231	-11.153	0.077	
70.32						
Ca	3.840e-02					
Ca+2	3.709e-02	8.829e-03	-1.431	-2.054	-0.623	-
16.37						
CaSO4	1.245e-03	1.487e-03	-2.905	-2.828	0.077	
7.96						
CaHCO3+	5.477e-05	3.721e-05	-4.261	-4.429	-0.168	
10.45						
CaCO3	1.090e-05	1.303e-05	-4.962	-4.885	0.077	-
14.56						
CaOH+	6.919e-08	5.206e-08	-7.160	-7.284	-0.124	
(0)						
CaHSO4+	4.545e-10	3.419e-10	-9.343	-9.466	-0.124	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.017e-01	-0.185	-0.396	-0.211	
19.13						
H(0)	7.795e-27					
H2	3.898e-27	4.658e-27	-26.409	-26.332	0.077	
28.59						
Mg	5.808e-02					
Mg+2	5.432e-02	1.516e-02	-1.265	-1.819	-0.554	-
20.73						
MgSO4	3.656e-03	4.370e-03	-2.437	-2.360	0.077	
6.30						
MgHCO3+	8.839e-05	5.412e-05	-4.054	-4.267	-0.213	
6.17						
MgOH+	1.025e-05	7.102e-06	-4.989	-5.149	-0.159	
(0)						
MgCO3	9.276e-06	1.109e-05	-5.033	-4.955	0.077	-
17.10						
Na	5.090e-01					
Na+	5.064e-01	3.608e-01	-0.296	-0.443	-0.147	
0.10						
NaSO4-	2.546e-03	1.685e-03	-2.594	-2.773	-0.179	
21.51						
NaHCO3	4.373e-05	5.226e-05	-4.359	-4.282	0.077	
1.80						
NaCO3-	1.117e-05	8.403e-06	-4.952	-5.076	-0.124	
4.67						

NaOH	3.140e-17	3.753e-17	-16.503	-16.426	0.077
(0)					
O(0)	1.251e-35				
O2	6.255e-36	7.475e-36	-35.204	-35.126	0.077
31.40					
S(6)	1.260e-02				
SO4-2	5.153e-03	8.511e-04	-2.288	-3.070	-0.782
19.46					
MgSO4	3.656e-03	4.370e-03	-2.437	-2.360	0.077
6.30					
NaSO4-	2.546e-03	1.685e-03	-2.594	-2.773	-0.179
21.51					
CaSO4	1.245e-03	1.487e-03	-2.905	-2.828	0.077
7.96					
HSO4-	4.281e-09	3.221e-09	-8.368	-8.492	-0.124
41.83					
CaHSO4+	4.545e-10	3.419e-10	-9.343	-9.466	-0.124
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.67	-5.12	-4.45	CaSO4
Aragonite	0.18	-8.27	-8.45	CaCO3
Calcite	0.31	-8.27	-8.58	CaCO3
CO2(g)	-3.18	-4.81	-1.63	CO2
Dolomite	1.12	-16.30	-17.42	CaMg(CO3)2
Gypsum	-0.55	-5.14	-4.60	CaSO4:2H2O
H2(g)	-23.20	-26.33	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-32.14	-35.13	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.126 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=25.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=25.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.56
pe 4
redox pe
units mmol/kgw
density 1
Ca 38.29
Mg 57.91
Na 509
S(6) 12.6
Alkalinity 0.655 as HCO3-
Cl 653
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	6.550e-04	6.550e-04
Ca	3.829e-02	3.829e-02
Cl	6.530e-01	6.530e-01
Mg	5.791e-02	5.791e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

pH = 7.560
pe = 4.000

Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C) = 75810
 Density (g/cm^3) = 1.01980
 Volume (L) = 1.01887
 Activity of water = 0.979
 Ionic strength (mol/kgw) = $7.739\text{e-}01$
 Mass of water (kg) = $1.000\text{e+}00$
 Total carbon (mol/kg) = $6.227\text{e-}04$
 Total CO_2 (mol/kg) = $6.227\text{e-}04$
 Temperature ($^\circ\text{C}$) = 40.00
 Electrical balance (eq) = $2.254\text{e-}02$
 Percent error, $100 * (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = 1.66
 Iterations = 7
 Total H = $1.110130\text{e+}02$
 Total O = $5.555848\text{e+}01$

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

--

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm^3/mol						
OH-	$1.760\text{e-}06$	$1.040\text{e-}06$	-5.754	-5.983	-0.228	-
2.02						
H+	$3.693\text{e-}08$	$2.754\text{e-}08$	-7.433	-7.560	-0.127	
0.00						
H ₂ O	$5.551\text{e+}01$	$9.785\text{e-}01$	1.744	-0.009	0.000	
18.16						
C(4)	$6.227\text{e-}04$					
HCO ₃ -	$4.006\text{e-}04$	$2.651\text{e-}04$	-3.397	-3.577	-0.179	
27.91						
MgHCO ₃ +	$8.365\text{e-}05$	$5.122\text{e-}05$	-4.078	-4.291	-0.213	
6.17						
CaHCO ₃ +	$5.184\text{e-}05$	$3.522\text{e-}05$	-4.285	-4.453	-0.168	
10.45						
NaHCO ₃	$4.151\text{e-}05$	$4.960\text{e-}05$	-4.382	-4.304	0.077	
1.80						
CO ₂	$1.238\text{e-}05$	$1.480\text{e-}05$	-4.907	-4.830	0.077	
35.16						
NaCO ₃ -	$1.060\text{e-}05$	$7.976\text{e-}06$	-4.975	-5.098	-0.124	
4.67						
CaCO ₃	$1.032\text{e-}05$	$1.234\text{e-}05$	-4.986	-4.909	0.077	-
14.56						
MgCO ₃	$8.780\text{e-}06$	$1.049\text{e-}05$	-5.057	-4.979	0.077	-
17.10						
CO ₃ -2	$3.011\text{e-}06$	$5.777\text{e-}07$	-5.521	-6.238	-0.717	-
1.44						
(CO ₂) ₂	$5.299\text{e-}12$	$6.333\text{e-}12$	-11.276	-11.198	0.077	
70.32						
Ca	$3.829\text{e-}02$					
Ca+2	$3.699\text{e-}02$	$8.804\text{e-}03$	-1.432	-2.055	-0.623	-
16.38						
CaSO ₄	$1.243\text{e-}03$	$1.485\text{e-}03$	-2.906	-2.828	0.077	
7.96						
CaHCO ₃ +	$5.184\text{e-}05$	$3.522\text{e-}05$	-4.285	-4.453	-0.168	
10.45						

CaCO3	1.032e-05	1.234e-05	-4.986	-4.909	0.077	-
14.56						
CaOH+	6.900e-08	5.191e-08	-7.161	-7.285	-0.124	
(0)						
CaHSO4+	4.538e-10	3.414e-10	-9.343	-9.467	-0.124	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.017e-01	-0.185	-0.396	-0.211	
19.13						
H(0)	7.796e-27					
H2	3.898e-27	4.658e-27	-26.409	-26.332	0.077	
28.59						
Mg	5.791e-02					
Mg+2	5.416e-02	1.512e-02	-1.266	-1.821	-0.554	-
20.73						
MgSO4	3.650e-03	4.362e-03	-2.438	-2.360	0.077	
6.30						
MgHCO3+	8.365e-05	5.122e-05	-4.078	-4.291	-0.213	
6.17						
MgOH+	1.022e-05	7.081e-06	-4.991	-5.150	-0.159	
(0)						
MgCO3	8.780e-06	1.049e-05	-5.057	-4.979	0.077	-
17.10						
Na	5.090e-01					
Na+	5.064e-01	3.608e-01	-0.296	-0.443	-0.147	
0.10						
NaSO4-	2.549e-03	1.687e-03	-2.594	-2.773	-0.179	
21.50						
NaHCO3	4.151e-05	4.960e-05	-4.382	-4.304	0.077	
1.80						
NaCO3-	1.060e-05	7.976e-06	-4.975	-5.098	-0.124	
4.67						
NaOH	3.140e-17	3.753e-17	-16.503	-16.426	0.077	
(0)						
O(0)	1.251e-35					
O2	6.255e-36	7.476e-36	-35.204	-35.126	0.077	
31.40						
S(6)	1.260e-02					
SO4-2	5.158e-03	8.522e-04	-2.288	-3.069	-0.782	
19.46						
MgSO4	3.650e-03	4.362e-03	-2.438	-2.360	0.077	
6.30						
NaSO4-	2.549e-03	1.687e-03	-2.594	-2.773	-0.179	
21.50						
CaSO4	1.243e-03	1.485e-03	-2.906	-2.828	0.077	
7.96						
HSO4-	4.287e-09	3.225e-09	-8.368	-8.491	-0.124	
41.83						
CaHSO4+	4.538e-10	3.414e-10	-9.343	-9.467	-0.124	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.67	-5.12	-4.45	CaSO4

Aragonite	0.15	-8.29	-8.45	CaCO3
Calcite	0.29	-8.29	-8.58	CaCO3
CO2(g)	-3.20	-4.83	-1.63	CO2
Dolomite	1.07	-16.35	-17.42	CaMg(CO3)2
Gypsum	-0.55	-5.14	-4.60	CaSO4:2H2O
H2(g)	-23.20	-26.33	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-32.14	-35.13	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.132 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=30.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=30.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat
SOLUTION 1
temp 40
pH 7.51
pe 4
redox pe

```

units      mmol/kgw
density    1
Ca         39.71
Mg         59.89
Na         509
S(6)      12.6
Alkalinity 0.7 as HCO3-
Cl         653
water     1 # kgg

```

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	7.000e-04	7.000e-04
Ca	3.971e-02	3.971e-02
Cl	6.530e-01	6.530e-01
Mg	5.989e-02	5.989e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

```

pH = 7.510
pe = 4.000
Specific Conductance (µS/cm, 40°C) = 75947
Density (g/cm³) = 1.01997
Volume (L) = 1.01881
Activity of water = 0.978
Ionic strength (mol/kgw) = 7.803e-01
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 6.719e-04
Total CO2 (mol/kg) = 6.719e-04
Temperature (°C) = 40.00
Electrical balance (eq) = 2.930e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 2.15
Iterations = 7
Total H = 1.110131e+02
Total O = 5.555863e+01

```

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

mole V Species cm ³ /mol	Molality	Activity	Log	Log	Log	-
			Molality	Activity	Gamma	
OH- 2.01	1.570e-06	9.271e-07	-5.804	-6.033	-0.229	-

H+	4.145e-08	3.090e-08	-7.382	-7.510	-0.128	
0.00						
H2O	5.551e+01	9.785e-01	1.744	-0.009	0.000	
18.16						
C(4)	6.719e-04					
HCO3-	4.300e-04	2.844e-04	-3.367	-3.546	-0.180	
27.93						
MgHCO3+	9.300e-05	5.690e-05	-4.032	-4.245	-0.213	
6.17						
CaHCO3+	5.771e-05	3.919e-05	-4.239	-4.407	-0.168	
10.45						
NaHCO3	4.447e-05	5.323e-05	-4.352	-4.274	0.078	
1.80						
CO2	1.488e-05	1.781e-05	-4.827	-4.749	0.078	
35.16						
CaCO3	1.022e-05	1.223e-05	-4.991	-4.913	0.078	-
14.56						
NaCO3-	1.013e-05	7.628e-06	-4.994	-5.118	-0.123	
4.70						
MgCO3	8.679e-06	1.039e-05	-5.062	-4.983	0.078	-
17.10						
CO3-2	2.886e-06	5.523e-07	-5.540	-6.258	-0.718	-
1.42						
(CO2)2	7.666e-12	9.175e-12	-11.115	-11.037	0.078	
70.32						
Ca	3.971e-02					
Ca+2	3.837e-02	9.131e-03	-1.416	-2.039	-0.624	-
16.37						
CaSO4	1.268e-03	1.517e-03	-2.897	-2.819	0.078	
7.96						
CaHCO3+	5.771e-05	3.919e-05	-4.239	-4.407	-0.168	
10.45						
CaCO3	1.022e-05	1.223e-05	-4.991	-4.913	0.078	-
14.56						
CaOH+	6.371e-08	4.798e-08	-7.196	-7.319	-0.123	
(0)						
CaHSO4+	5.196e-10	3.914e-10	-9.284	-9.407	-0.123	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.014e-01	-0.185	-0.396	-0.211	
19.14						
H(0)	9.800e-27					
H2	4.900e-27	5.865e-27	-26.310	-26.232	0.078	
28.59						
Mg	5.989e-02					
Mg+2	5.606e-02	1.565e-02	-1.251	-1.805	-0.554	-
20.73						
MgSO4	3.719e-03	4.451e-03	-2.430	-2.352	0.078	
6.30						
MgHCO3+	9.300e-05	5.690e-05	-4.032	-4.245	-0.213	
6.17						
MgOH+	9.438e-06	6.535e-06	-5.025	-5.185	-0.160	
(0)						
MgCO3	8.679e-06	1.039e-05	-5.062	-4.983	0.078	-
17.10						
Na	5.090e-01					

Na+	5.064e-01	3.609e-01	-0.295	-0.443	-0.147
0.11					
NaSO4-	2.514e-03	1.662e-03	-2.600	-2.779	-0.180
21.54					
NaHCO3	4.447e-05	5.323e-05	-4.352	-4.274	0.078
1.80					
NaCO3-	1.013e-05	7.628e-06	-4.994	-5.118	-0.123
4.70					
NaOH	2.795e-17	3.346e-17	-16.554	-16.476	0.078
(0)					
O(0)	7.881e-36				
O2	3.941e-36	4.716e-36	-35.404	-35.326	0.078
31.40					
S(6)	1.260e-02				
SO4-2	5.100e-03	8.396e-04	-2.292	-3.076	-0.784
19.47					
MgSO4	3.719e-03	4.451e-03	-2.430	-2.352	0.078
6.30					
NaSO4-	2.514e-03	1.662e-03	-2.600	-2.779	-0.180
21.54					
CaSO4	1.268e-03	1.517e-03	-2.897	-2.819	0.078
7.96					
HSO4-	4.734e-09	3.565e-09	-8.325	-8.448	-0.123
41.84					
CaHSO4+	5.196e-10	3.914e-10	-9.284	-9.407	-0.123
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.66	-5.12	-4.45	CaSO4
Aragonite	0.15	-8.30	-8.45	CaCO3
Calcite	0.28	-8.30	-8.58	CaCO3
CO2(g)	-3.12	-4.75	-1.63	CO2
Dolomite	1.06	-16.36	-17.42	CaMg(CO3)2
Gypsum	-0.54	-5.13	-4.60	CaSO4:2H2O
H2(g)	-23.10	-26.23	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-32.34	-35.33	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.128 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=80.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\SP\sp_ID=80.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.56
pe 4
redox pe
units mmol/kgw
density 1
Ca 44.28
Mg 67.06
Na 509
S(6) 12.6
Alkalinity 0.6 as HCO3-
Cl 653
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	6.000e-04	6.000e-04
Ca	4.428e-02	4.428e-02
Cl	6.530e-01	6.530e-01
Mg	6.706e-02	6.706e-02

Na 5.090e-01 5.090e-01
 S(6) 1.260e-02 1.260e-02

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

pH = 7.560
 pe = 4.000
 Specific Conductance (µS/cm, 40°C) = 76414
 Density (g/cm³) = 1.02052
 Volume (L) = 1.01860
 Activity of water = 0.978
 Ionic strength (mol/kgw) = 8.028e-01
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 5.659e-04
 Total CO2 (mol/kg) = 5.659e-04
 Temperature (°C) = 40.00
 Electrical balance (eq) = 5.288e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 3.82
 Iterations = 7
 Total H = 1.110130e+02
 Total O = 5.555832e+01

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

mole V Species cm³/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH- 1.97	1.768e-06	1.040e-06	-5.753	-5.983	-0.230	-
H+ 0.00	3.698e-08	2.754e-08	-7.432	-7.560	-0.128	
H2O 18.16	5.551e+01	9.783e-01	1.744	-0.010	0.000	
C(4) 27.99	5.659e-04					
HCO3- 6.18	3.503e-04	2.312e-04	-3.456	-3.636	-0.181	
MgHCO3+ 10.45	8.535e-05	5.205e-05	-4.069	-4.284	-0.215	
CaHCO3+ 1.80	5.244e-05	3.554e-05	-4.280	-4.449	-0.169	
NaHCO3 35.16	3.601e-05	4.333e-05	-4.444	-4.363	0.080	
CO2 14.56	1.073e-05	1.291e-05	-4.969	-4.889	0.080	
CaCO3 4.83	1.035e-05	1.245e-05	-4.985	-4.905	0.080	-
NaCO3- 17.10	9.214e-06	6.966e-06	-5.036	-5.157	-0.121	
MgCO3 1.37	8.862e-06	1.066e-05	-5.052	-4.972	0.080	-
CO3-2	2.657e-06	5.037e-07	-5.576	-6.298	-0.722	-

(CO2)2	4.004e-12	4.817e-12	-11.397	-11.317	0.080	
70.32						
Ca	4.428e-02					
Ca+2	4.288e-02	1.019e-02	-1.368	-1.992	-0.624	-
16.35						
CaSO4	1.338e-03	1.609e-03	-2.874	-2.793	0.080	
7.96						
CaHCO3+	5.244e-05	3.554e-05	-4.280	-4.449	-0.169	
10.45						
CaCO3	1.035e-05	1.245e-05	-4.985	-4.905	0.080	-
14.56						
CaOH+	7.943e-08	6.006e-08	-7.100	-7.221	-0.121	
(0)						
CaHSO4+	4.893e-10	3.700e-10	-9.310	-9.432	-0.121	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.003e-01	-0.185	-0.398	-0.213	
19.15						
H(0)	7.744e-27					
H2	3.872e-27	4.658e-27	-26.412	-26.332	0.080	
28.59						
Mg	6.706e-02					
Mg+2	6.300e-02	1.762e-02	-1.201	-1.754	-0.553	-
20.71						
MgSO4	3.958e-03	4.761e-03	-2.403	-2.322	0.080	
6.30						
MgHCO3+	8.535e-05	5.205e-05	-4.069	-4.284	-0.215	
6.18						
MgOH+	1.194e-05	8.250e-06	-4.923	-5.084	-0.160	
(0)						
MgCO3	8.862e-06	1.066e-05	-5.052	-4.972	0.080	-
17.10						
Na	5.090e-01					
Na+	5.066e-01	3.614e-01	-0.295	-0.442	-0.147	
0.12						
NaSO4-	2.398e-03	1.582e-03	-2.620	-2.801	-0.181	
21.67						
NaHCO3	3.601e-05	4.333e-05	-4.444	-4.363	0.080	
1.80						
NaCO3-	9.214e-06	6.966e-06	-5.036	-5.157	-0.121	
4.83						
NaOH	3.124e-17	3.758e-17	-16.505	-16.425	0.080	
(0)						
O(0)	1.242e-35					
O2	6.211e-36	7.472e-36	-35.207	-35.127	0.080	
31.40						
S(6)	1.260e-02					
SO4-2	4.907e-03	7.981e-04	-2.309	-3.098	-0.789	
19.53						
MgSO4	3.958e-03	4.761e-03	-2.403	-2.322	0.080	
6.30						
NaSO4-	2.398e-03	1.582e-03	-2.620	-2.801	-0.181	
21.67						
CaSO4	1.338e-03	1.609e-03	-2.874	-2.793	0.080	
7.96						
HSO4-	3.995e-09	3.020e-09	-8.398	-8.520	-0.121	
41.85						

CaHSO4+ 4.893e-10 3.700e-10 -9.310 -9.432 -0.121
(0)

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.64	-5.09	-4.45	CaSO4
Aragonite	0.16	-8.29	-8.45	CaCO3
Calcite	0.29	-8.29	-8.58	CaCO3
CO2(g)	-3.26	-4.89	-1.63	CO2
Dolomite	1.08	-16.34	-17.42	CaMg(CO3)2
Gypsum	-0.51	-5.11	-4.60	CaSO4:2H2O
H2(g)	-23.20	-26.33	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-32.14	-35.13	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.132 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=0.5.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=0.5.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35.98
Mg 55.05
Na 509
S(6) 12.6
Alkalinity 0.8 as HCO3-
Cl 653
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	8.000e-04	8.000e-04
Ca	3.598e-02	3.598e-02
Cl	6.530e-01	6.530e-01
Mg	5.505e-02	5.505e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	75597
Density (g/cm^3)	=	1.01956
Volume (L)	=	1.01896
Activity of water	=	0.979
Ionic strength (mol/kgw)	=	7.639e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	6.298e-04
Total CO2 (mol/kg)	=	6.298e-04
Temperature (°C)	=	40.00
Electrical balance (eq)	=	1.206e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	0.90
Iterations	=	6
Total H	=	1.110130e+02
Total O	=	5.555855e+01

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

--

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	7.670e-06	4.541e-06	-5.115	-5.343	-0.228	-
2.04						
H+	8.455e-09	6.310e-09	-8.073	-8.200	-0.127	
0.00						
H2O	5.551e+01	9.786e-01	1.744	-0.009	0.000	
18.16						
C(4)	6.298e-04					
HCO3-	3.546e-04	2.350e-04	-3.450	-3.629	-0.179	
27.89						
MgHCO3+	7.016e-05	4.303e-05	-4.154	-4.366	-0.212	
6.17						
CaHCO3+	4.311e-05	2.932e-05	-4.365	-4.533	-0.167	
10.45						
NaCO3-	4.106e-05	3.084e-05	-4.387	-4.511	-0.124	
4.61						
CaCO3	3.759e-05	4.481e-05	-4.425	-4.349	0.076	-
14.56						
NaHCO3	3.685e-05	4.394e-05	-4.434	-4.357	0.076	
1.80						
MgCO3	3.227e-05	3.847e-05	-4.491	-4.415	0.076	-
17.10						
CO3-2	1.160e-05	2.235e-06	-4.935	-5.651	-0.715	-
1.46						
CO2	2.520e-06	3.005e-06	-5.599	-5.522	0.076	
35.16						
(CO2)2	2.189e-13	2.610e-13	-12.660	-12.583	0.076	
70.32						
Ca	3.598e-02					
Ca+2	3.470e-02	8.267e-03	-1.460	-2.083	-0.623	-
16.38						
CaSO4	1.197e-03	1.427e-03	-2.922	-2.846	0.076	
7.96						
CaHCO3+	4.311e-05	2.932e-05	-4.365	-4.533	-0.167	
10.45						
CaCO3	3.759e-05	4.481e-05	-4.425	-4.349	0.076	-
14.56						
CaOH+	2.833e-07	2.128e-07	-6.548	-6.672	-0.124	
(0)						
CaHSO4+	1.001e-10	7.515e-11	-10.000	-10.124	-0.124	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.022e-01	-0.185	-0.396	-0.210	
19.13						
H(0)	4.101e-28					
H2	2.050e-28	2.445e-28	-27.688	-27.612	0.076	
28.59						
Mg	5.505e-02					
Mg+2	5.136e-02	1.433e-02	-1.289	-1.844	-0.554	-
20.74						

MgSO4	3.549e-03	4.231e-03	-2.450	-2.374	0.076	
6.30						
MgHCO3+	7.016e-05	4.303e-05	-4.154	-4.366	-0.212	
6.17						
MgOH+	4.226e-05	2.930e-05	-4.374	-4.533	-0.159	
(0)						
MgCO3	3.227e-05	3.847e-05	-4.491	-4.415	0.076	-
17.10						
Na	5.090e-01					
Na+	5.063e-01	3.605e-01	-0.296	-0.443	-0.147	
0.10						
NaSO4-	2.604e-03	1.725e-03	-2.584	-2.763	-0.179	
21.44						
NaCO3-	4.106e-05	3.084e-05	-4.387	-4.511	-0.124	
4.61						
NaHCO3	3.685e-05	4.394e-05	-4.434	-4.357	0.076	
1.80						
NaOH	1.373e-16	1.637e-16	-15.862	-15.786	0.076	
(0)						
O(0)	4.554e-33					
O2	2.277e-33	2.715e-33	-32.643	-32.566	0.076	
31.40						
S(6)	1.260e-02					
SO4-2	5.250e-03	8.721e-04	-2.280	-3.059	-0.780	
19.43						
MgSO4	3.549e-03	4.231e-03	-2.450	-2.374	0.076	
6.30						
NaSO4-	2.604e-03	1.725e-03	-2.584	-2.763	-0.179	
21.44						
CaSO4	1.197e-03	1.427e-03	-2.922	-2.846	0.076	
7.96						
HSO4-	1.007e-09	7.561e-10	-8.997	-9.121	-0.124	
41.83						
CaHSO4+	1.001e-10	7.515e-11	-10.000	-10.124	-0.124	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.69	-5.14	-4.45	CaSO4
Aragonite	0.71	-7.73	-8.45	CaCO3
Calcite	0.85	-7.73	-8.58	CaCO3
CO2(g)	-3.90	-5.52	-1.63	CO2
Dolomite	2.19	-15.23	-17.42	CaMg(CO3)2
Gypsum	-0.56	-5.16	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-29.58	-32.57	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

Reading input data for simulation 2.

End of Run after 0.139 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=1.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=1.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat
SOLUTION 1
temp 40
pH 7.79
pe 4
redox pe
units mmol/kgw
density 1
Ca 33.99
Mg 52.30
Na 509
S(6) 12.6
Alkalinity 0.685 as HCO3-
Cl 653
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

--

Elements	Molality	Moles
Alkalinity	6.850e-04	6.850e-04
Ca	3.399e-02	3.399e-02
Cl	6.530e-01	6.530e-01
Mg	5.230e-02	5.230e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

--

pH	=	7.790
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	75406
Density (g/cm^3)	=	1.01933
Volume (L)	=	1.01904
Activity of water	=	0.979
Ionic strength (mol/kgw)	=	7.550e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	6.215e-04
Total CO2 (mol/kg)	=	6.215e-04
Temperature (°C)	=	40.00
Electrical balance (eq)	=	2.695e-03
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	0.20
Iterations	=	6
Total H	=	1.110130e+02
Total O	=	5.555849e+01

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	2.980e-06	1.767e-06	-5.526	-5.753	-0.227	-
2.06						
H+	2.172e-08	1.622e-08	-7.663	-7.790	-0.127	
0.00						
H2O	5.551e+01	9.787e-01	1.744	-0.009	0.000	
18.16						
C(4)	6.215e-04					
HCO3-	3.995e-04	2.649e-04	-3.398	-3.577	-0.178	
27.86						
MgHCO3+	7.497e-05	4.603e-05	-4.125	-4.337	-0.212	
6.17						
CaHCO3+	4.590e-05	3.124e-05	-4.338	-4.505	-0.167	
10.45						
NaHCO3	4.162e-05	4.952e-05	-4.381	-4.305	0.075	
1.80						
NaCO3-	1.803e-05	1.352e-05	-4.744	-4.869	-0.125	
4.56						

CaCO3	1.561e-05	1.858e-05	-4.806	-4.731	0.075	-
14.56						
MgCO3	1.346e-05	1.601e-05	-4.871	-4.795	0.075	-
17.10						
CO2	7.318e-06	8.708e-06	-5.136	-5.060	0.075	
35.16						
CO3-2	5.070e-06	9.805e-07	-5.295	-6.009	-0.714	-
1.48						
(CO2)2	1.843e-12	2.192e-12	-11.735	-11.659	0.075	
70.32						
Ca	3.399e-02					
Ca+2	3.277e-02	7.813e-03	-1.485	-2.107	-0.623	-
16.39						
CaSO4	1.158e-03	1.378e-03	-2.936	-2.861	0.075	
7.96						
CaHCO3+	4.590e-05	3.124e-05	-4.338	-4.505	-0.167	
10.45						
CaCO3	1.561e-05	1.858e-05	-4.806	-4.731	0.075	-
14.56						
CaOH+	1.043e-07	7.825e-08	-6.982	-7.107	-0.125	
(0)						
CaHSO4+	2.487e-10	1.865e-10	-9.604	-9.729	-0.125	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.027e-01	-0.185	-0.395	-0.210	
19.12						
H(0)	2.715e-27					
H2	1.358e-27	1.615e-27	-26.867	-26.792	0.075	
28.59						
Mg	5.230e-02					
Mg+2	4.875e-02	1.359e-02	-1.312	-1.867	-0.555	-
20.75						
MgSO4	3.448e-03	4.102e-03	-2.462	-2.387	0.075	
6.30						
MgHCO3+	7.497e-05	4.603e-05	-4.125	-4.337	-0.212	
6.17						
MgOH+	1.559e-05	1.082e-05	-4.807	-4.966	-0.159	
(0)						
MgCO3	1.346e-05	1.601e-05	-4.871	-4.795	0.075	-
17.10						
Na	5.090e-01					
Na+	5.063e-01	3.604e-01	-0.296	-0.443	-0.148	
0.09						
NaSO4-	2.657e-03	1.762e-03	-2.576	-2.754	-0.178	
21.39						
NaHCO3	4.162e-05	4.952e-05	-4.381	-4.305	0.075	
1.80						
NaCO3-	1.803e-05	1.352e-05	-4.744	-4.869	-0.125	
4.56						
NaOH	5.351e-17	6.367e-17	-16.272	-16.196	0.075	
(0)						
O(0)	1.045e-34					
O2	5.227e-35	6.220e-35	-34.282	-34.206	0.075	
31.40						
S(6)	1.260e-02					
SO4-2	5.337e-03	8.911e-04	-2.273	-3.050	-0.777	
19.41						

MgSO4	3.448e-03	4.102e-03	-2.462	-2.387	0.075
6.30					
NaSO4-	2.657e-03	1.762e-03	-2.576	-2.754	-0.178
21.39					
CaSO4	1.158e-03	1.378e-03	-2.936	-2.861	0.075
7.96					
HSO4-	2.648e-09	1.986e-09	-8.577	-8.702	-0.125
41.82					
CaHSO4+	2.487e-10	1.865e-10	-9.604	-9.729	-0.125
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.71	-5.16	-4.45	CaSO4
Aragonite	0.33	-8.12	-8.45	CaCO3
Calcite	0.46	-8.12	-8.58	CaCO3
CO2 (g)	-3.44	-5.06	-1.63	CO2
Dolomite	1.43	-15.99	-17.42	CaMg(CO3)2
Gypsum	-0.58	-5.18	-4.60	CaSO4:2H2O
H2 (g)	-23.66	-26.79	-3.13	H2
H2O (g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2 (g)	-31.22	-34.21	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.032 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=2.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=2.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.75
pe 4
redox pe
units mmol/kgw
density 1
Ca 37.2151055814039
Mg 56.68055956
Na 509
S(6) 12.6
Alkalinity 0.82 as HCO3-
Cl 653
water 1 # kgw

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	8.200e-04	8.200e-04
Ca	3.722e-02	3.722e-02
Cl	6.530e-01	6.530e-01
Mg	5.668e-02	5.668e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

pH	=	7.750
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	75715
Density (g/cm^3)	=	1.01970
Volume (L)	=	1.01891
Activity of water	=	0.979
Ionic strength (mol/kgw)	=	7.694e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	7.518e-04
Total CO2 (mol/kg)	=	7.518e-04

Temperature (°C) = 40.00
 Electrical balance (eq) = 1.777e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.32
 Iterations = 7
 Total H = 1.110131e+02
 Total O = 5.555888e+01

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

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	2.724e-06	1.611e-06	-5.565	-5.793	-0.228	-
2.03						
H+	2.384e-08	1.778e-08	-7.623	-7.750	-0.127	
0.00						
H2O	5.551e+01	9.786e-01	1.744	-0.009	0.000	
18.16						
C(4)	7.518e-04					
HCO3-	4.764e-04	3.154e-04	-3.322	-3.501	-0.179	
27.90						
MgHCO3+	9.721e-05	5.956e-05	-4.012	-4.225	-0.213	
6.17						
CaHCO3+	5.990e-05	4.071e-05	-4.223	-4.390	-0.168	
10.45						
NaHCO3	4.942e-05	5.900e-05	-4.306	-4.229	0.077	
1.80						
NaCO3-	1.955e-05	1.469e-05	-4.709	-4.833	-0.124	
4.64						
CaCO3	1.850e-05	2.208e-05	-4.733	-4.656	0.077	-
14.56						
MgCO3	1.583e-05	1.890e-05	-4.801	-4.724	0.077	-
17.10						
CO2	9.523e-06	1.137e-05	-5.021	-4.944	0.077	
35.16						
CO3-2	5.539e-06	1.065e-06	-5.257	-5.973	-0.716	-
1.45						
(CO2)2	3.130e-12	3.737e-12	-11.504	-11.427	0.077	
70.32						
Ca	3.722e-02					
Ca+2	3.592e-02	8.553e-03	-1.445	-2.068	-0.623	-
16.38						
CaSO4	1.221e-03	1.457e-03	-2.913	-2.836	0.077	
7.96						
CaHCO3+	5.990e-05	4.071e-05	-4.223	-4.390	-0.168	
10.45						
CaCO3	1.850e-05	2.208e-05	-4.733	-4.656	0.077	-
14.56						
CaOH+	1.039e-07	7.811e-08	-6.983	-7.107	-0.124	
(0)						
CaHSO4+	2.877e-10	2.163e-10	-9.541	-9.665	-0.124	
(0)						
Cl	6.530e-01					

Cl-	6.530e-01	4.019e-01	-0.185	-0.396	-0.211	
19.13						
H(0)	3.253e-27					
H2	1.627e-27	1.942e-27	-26.789	-26.712	0.077	
28.59						
Mg	5.668e-02					
Mg+2	5.294e-02	1.477e-02	-1.276	-1.830	-0.554	-
20.74						
MgSO4	3.608e-03	4.307e-03	-2.443	-2.366	0.077	
6.30						
MgHCO3+	9.721e-05	5.956e-05	-4.012	-4.225	-0.213	
6.17						
MgCO3	1.583e-05	1.890e-05	-4.801	-4.724	0.077	-
17.10						
MgOH+	1.547e-05	1.072e-05	-4.811	-4.970	-0.159	
(0)						
Na	5.090e-01					
Na+	5.064e-01	3.607e-01	-0.296	-0.443	-0.147	
0.10						
NaSO4-	2.573e-03	1.704e-03	-2.590	-2.769	-0.179	
21.48						
NaHCO3	4.942e-05	5.900e-05	-4.306	-4.229	0.077	
1.80						
NaCO3-	1.955e-05	1.469e-05	-4.709	-4.833	-0.124	
4.64						
NaOH	4.867e-17	5.811e-17	-16.313	-16.236	0.077	
(0)						
O(0)	7.207e-35					
O2	3.604e-35	4.302e-35	-34.443	-34.366	0.077	
31.40						
S(6)	1.260e-02					
SO4-2	5.198e-03	8.609e-04	-2.284	-3.065	-0.781	
19.45						
MgSO4	3.608e-03	4.307e-03	-2.443	-2.366	0.077	
6.30						
NaSO4-	2.573e-03	1.704e-03	-2.590	-2.769	-0.179	
21.48						
CaSO4	1.221e-03	1.457e-03	-2.913	-2.836	0.077	
7.96						
HSO4-	2.798e-09	2.104e-09	-8.553	-8.677	-0.124	
41.83						
CaHSO4+	2.877e-10	2.163e-10	-9.541	-9.665	-0.124	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.68	-5.13	-4.45	CaSO4
Aragonite	0.41	-8.04	-8.45	CaCO3
Calcite	0.54	-8.04	-8.58	CaCO3
CO2(g)	-3.32	-4.94	-1.63	CO2
Dolomite	1.58	-15.84	-17.42	CaMg(CO3)2
Gypsum	-0.56	-5.15	-4.60	CaSO4:2H2O
H2(g)	-23.58	-26.71	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O

Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-31.38	-34.37	-2.98	O2

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.028 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=5.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=5.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.6
pe 4
redox pe
units mmol/kgw
density 1
Ca 39.3445277
Mg 59.7724748
Na 509
S(6) 12.6
Alkalinity 0.88 as HCO3-

Cl 653
 water 1 # kgg

 Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	8.800e-04	8.800e-04
Ca	3.934e-02	3.934e-02
Cl	6.530e-01	6.530e-01
Mg	5.977e-02	5.977e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

pH = 7.600
 pe = 4.000
 Specific Conductance (µS/cm, 40°C) = 75926
 Density (g/cm³) = 1.01995
 Volume (L) = 1.01882
 Activity of water = 0.978
 Ionic strength (mol/kgw) = 7.794e-01
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 8.331e-04
 Total CO2 (mol/kg) = 8.331e-04
 Temperature (°C) = 40.00
 Electrical balance (eq) = 2.815e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 2.07
 Iterations = 7
 Total H = 1.110132e+02
 Total O = 5.555911e+01

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

mole V Species cm³/mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.931e-06	1.141e-06	-5.714	-5.943	-0.229	-
2.01 H+	3.369e-08	2.512e-08	-7.473	-7.600	-0.127	
0.00 H2O	5.551e+01	9.785e-01	1.744	-0.009	0.000	
18.16 C(4)	8.331e-04					
HCO3-	5.302e-04	3.507e-04	-3.276	-3.455	-0.180	
27.93						

MgHCO3+	1.144e-04	6.999e-05	-3.942	-4.155	-0.213	
6.17						
CaHCO3+	7.048e-05	4.786e-05	-4.152	-4.320	-0.168	
10.45						
NaHCO3	5.486e-05	6.564e-05	-4.261	-4.183	0.078	
1.80						
NaCO3-	1.537e-05	1.157e-05	-4.813	-4.937	-0.123	
4.70						
CaCO3	1.536e-05	1.838e-05	-4.814	-4.736	0.078	-
14.56						
CO2	1.492e-05	1.786e-05	-4.826	-4.748	0.078	
35.16						
MgCO3	1.314e-05	1.572e-05	-4.881	-4.804	0.078	-
17.10						
CO3-2	4.378e-06	8.381e-07	-5.359	-6.077	-0.718	-
1.42						
(CO2) 2	7.706e-12	9.220e-12	-11.113	-11.035	0.078	
70.32						
Ca	3.934e-02					
Ca+2	3.800e-02	9.042e-03	-1.420	-2.044	-0.624	-
16.37						
CaSO4	1.258e-03	1.506e-03	-2.900	-2.822	0.078	
7.96						
CaHCO3+	7.048e-05	4.786e-05	-4.152	-4.320	-0.168	
10.45						
CaCO3	1.536e-05	1.838e-05	-4.814	-4.736	0.078	-
14.56						
CaOH+	7.763e-08	5.846e-08	-7.110	-7.233	-0.123	
(0)						
CaHSO4+	4.192e-10	3.156e-10	-9.378	-9.501	-0.123	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.014e-01	-0.185	-0.396	-0.211	
19.14						
H(0)	6.476e-27					
H2	3.238e-27	3.875e-27	-26.490	-26.412	0.078	
28.59						
Mg	5.977e-02					
Mg+2	5.592e-02	1.561e-02	-1.252	-1.807	-0.554	-
20.73						
MgSO4	3.717e-03	4.447e-03	-2.430	-2.352	0.078	
6.30						
MgHCO3+	1.144e-04	6.999e-05	-3.942	-4.155	-0.213	
6.17						
MgCO3	1.314e-05	1.572e-05	-4.881	-4.804	0.078	-
17.10						
MgOH+	1.158e-05	8.018e-06	-4.936	-5.096	-0.160	
(0)						
Na	5.090e-01					
Na+	5.064e-01	3.609e-01	-0.295	-0.443	-0.147	
0.11						
NaSO4-	2.518e-03	1.666e-03	-2.599	-2.778	-0.180	
21.53						
NaHCO3	5.486e-05	6.564e-05	-4.261	-4.183	0.078	
1.80						
NaCO3-	1.537e-05	1.157e-05	-4.813	-4.937	-0.123	
4.70						

NaOH	3.440e-17	4.116e-17	-16.463	-16.386	0.078
(0)					
O(0)	1.806e-35				
O2	9.029e-36	1.080e-35	-35.044	-34.966	0.078
31.40					
S(6)	1.260e-02				
SO4-2	5.107e-03	8.412e-04	-2.292	-3.075	-0.783
19.47					
MgSO4	3.717e-03	4.447e-03	-2.430	-2.352	0.078
6.30					
NaSO4-	2.518e-03	1.666e-03	-2.599	-2.778	-0.180
21.53					
CaSO4	1.258e-03	1.506e-03	-2.900	-2.822	0.078
7.96					
HSO4-	3.856e-09	2.903e-09	-8.414	-8.537	-0.123
41.84					
CaHSO4+	4.192e-10	3.156e-10	-9.378	-9.501	-0.123
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.67	-5.12	-4.45	CaSO4
Aragonite	0.33	-8.12	-8.45	CaCO3
Calcite	0.46	-8.12	-8.58	CaCO3
CO2(g)	-3.12	-4.75	-1.63	CO2
Dolomite	1.42	-16.00	-17.42	CaMg(CO3)2
Gypsum	-0.54	-5.14	-4.60	CaSO4:2H2O
H2(g)	-23.28	-26.41	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-31.98	-34.97	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.136 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=10.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=10.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.53
pe 4
redox pe
units mmol/kgw
density 1
Ca 39.14506743
Mg 59.49812796
Na 509
S(6) 12.6
Alkalinity 0.66 as HCO3-
Cl 653
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	6.600e-04	6.600e-04
Ca	3.915e-02	3.915e-02
Cl	6.530e-01	6.530e-01
Mg	5.950e-02	5.950e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

pH = 7.530
pe = 4.000

Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C) = 75906
 Density (g/cm^3) = 1.01992
 Volume (L) = 1.01883
 Activity of water = 0.978
 Ionic strength (mol/kgw) = $7.785\text{e-}01$
 Mass of water (kg) = $1.000\text{e+}00$
 Total carbon (mol/kg) = $6.307\text{e-}04$
 Total CO_2 (mol/kg) = $6.307\text{e-}04$
 Temperature ($^\circ\text{C}$) = 40.00
 Electrical balance (eq) = $2.743\text{e-}02$
 Percent error, $100 * (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = 2.02
 Iterations = 7
 Total H = $1.110130\text{e+}02$
 Total O = $5.555851\text{e+}01$

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

--

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm^3/mol						
OH-	$1.644\text{e-}06$	$9.708\text{e-}07$	-5.784	-6.013	-0.229	-
2.01						
H+	$3.958\text{e-}08$	$2.951\text{e-}08$	-7.403	-7.530	-0.127	
0.00						
H ₂ O	$5.551\text{e+}01$	$9.785\text{e-}01$	1.744	-0.009	0.000	
18.16						
C(4)	$6.307\text{e-}04$					
HCO ₃ -	$4.040\text{e-}04$	$2.673\text{e-}04$	-3.394	-3.573	-0.179	
27.93						
MgHCO ₃ +	$8.679\text{e-}05$	$5.311\text{e-}05$	-4.062	-4.275	-0.213	
6.17						
CaHCO ₃ +	$5.346\text{e-}05$	$3.631\text{e-}05$	-4.272	-4.440	-0.168	
10.45						
NaHCO ₃	$4.181\text{e-}05$	$5.002\text{e-}05$	-4.379	-4.301	0.078	
1.80						
CO ₂	$1.336\text{e-}05$	$1.599\text{e-}05$	-4.874	-4.796	0.078	
35.16						
NaCO ₃ -	$9.970\text{e-}06$	$7.506\text{e-}06$	-5.001	-5.125	-0.123	
4.70						
CaCO ₃	$9.919\text{e-}06$	$1.187\text{e-}05$	-5.004	-4.926	0.078	-
14.56						
MgCO ₃	$8.487\text{e-}06$	$1.015\text{e-}05$	-5.071	-4.993	0.078	-
17.10						
CO ₃ -2	$2.839\text{e-}06$	$5.436\text{e-}07$	-5.547	-6.265	-0.718	-
1.43						
(CO ₂) ₂	$6.178\text{e-}12$	$7.391\text{e-}12$	-11.209	-11.131	0.078	
70.32						
Ca	$3.915\text{e-}02$					
Ca+2	$3.783\text{e-}02$	$9.002\text{e-}03$	-1.422	-2.046	-0.623	-
16.37						
CaSO ₄	$1.255\text{e-}03$	$1.502\text{e-}03$	-2.901	-2.823	0.078	
7.96						
CaHCO ₃ +	$5.346\text{e-}05$	$3.631\text{e-}05$	-4.272	-4.440	-0.168	
10.45						

CaCO3	9.919e-06	1.187e-05	-5.004	-4.926	0.078	-
14.56						
CaOH+	6.579e-08	4.953e-08	-7.182	-7.305	-0.123	
(0)						
CaHSO4+	4.912e-10	3.698e-10	-9.309	-9.432	-0.123	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.015e-01	-0.185	-0.396	-0.211	
19.14						
H(0)	8.942e-27					
H2	4.471e-27	5.349e-27	-26.350	-26.272	0.078	
28.59						
Mg	5.950e-02					
Mg+2	5.568e-02	1.555e-02	-1.254	-1.808	-0.554	-
20.73						
MgSO4	3.709e-03	4.437e-03	-2.431	-2.353	0.078	
6.30						
MgHCO3+	8.679e-05	5.311e-05	-4.062	-4.275	-0.213	
6.17						
MgOH+	9.814e-06	6.796e-06	-5.008	-5.168	-0.160	
(0)						
MgCO3	8.487e-06	1.015e-05	-5.071	-4.993	0.078	-
17.10						
Na	5.090e-01					
Na+	5.064e-01	3.609e-01	-0.295	-0.443	-0.147	
0.11						
NaSO4-	2.522e-03	1.669e-03	-2.598	-2.778	-0.179	
21.53						
NaHCO3	4.181e-05	5.002e-05	-4.379	-4.301	0.078	
1.80						
NaCO3-	9.970e-06	7.506e-06	-5.001	-5.125	-0.123	
4.70						
NaOH	2.928e-17	3.503e-17	-16.533	-16.456	0.078	
(0)						
O(0)	9.479e-36					
O2	4.740e-36	5.670e-36	-35.324	-35.246	0.078	
31.40						
S(6)	1.260e-02					
SO4-2	5.114e-03	8.427e-04	-2.291	-3.074	-0.783	
19.47						
MgSO4	3.709e-03	4.437e-03	-2.431	-2.353	0.078	
6.30						
NaSO4-	2.522e-03	1.669e-03	-2.598	-2.778	-0.179	
21.53						
CaSO4	1.255e-03	1.502e-03	-2.901	-2.823	0.078	
7.96						
HSO4-	4.539e-09	3.417e-09	-8.343	-8.466	-0.123	
41.84						
CaHSO4+	4.912e-10	3.698e-10	-9.309	-9.432	-0.123	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.67	-5.12	-4.45	CaSO4

Aragonite	0.14	-8.31	-8.45	CaCO3
Calcite	0.27	-8.31	-8.58	CaCO3
CO2(g)	-3.17	-4.80	-1.63	CO2
Dolomite	1.04	-16.38	-17.42	CaMg(CO3)2
Gypsum	-0.54	-5.14	-4.60	CaSO4:2H2O
H2(g)	-23.14	-26.27	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-32.26	-35.25	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.136 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=15.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=15.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat
SOLUTION 1
temp 40
pH 7.63
pe 4
redox pe

```

units      mmol/kgw
density    1
Ca         38.58031781
Mg         58.65056573
Na         509
S(6)      12.6
Alkalinity 0.6 as HCO3-
Cl         653
water     1 # kgg

```

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	6.000e-04	6.000e-04
Ca	3.858e-02	3.858e-02
Cl	6.530e-01	6.530e-01
Mg	5.865e-02	5.865e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

```

pH = 7.630
pe = 4.000
Specific Conductance (µS/cm, 40°C) = 75849
Density (g/cm³) = 1.01985
Volume (L) = 1.01885
Activity of water = 0.978
Ionic strength (mol/kgw) = 7.758e-01
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 5.606e-04
Total CO2 (mol/kg) = 5.606e-04
Temperature (°C) = 40.00
Electrical balance (eq) = 2.466e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.82
Iterations = 7
Total H = 1.110130e+02
Total O = 5.555830e+01

```

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

mole V Species cm ³ /mol	Molality	Activity	Log	Log	Log	-
			Molality	Activity	Gamma	
OH- 2.02	2.068e-06	1.222e-06	-5.684	-5.913	-0.229	-

H+	3.143e-08	2.344e-08	-7.503	-7.630	-0.127	
0.00						
H2O	5.551e+01	9.785e-01	1.744	-0.009	0.000	
18.16						
C(4)	5.606e-04					
HCO3-	3.574e-04	2.365e-04	-3.447	-3.626	-0.179	
27.92						
MgHCO3+	7.565e-05	4.631e-05	-4.121	-4.334	-0.213	
6.17						
CaHCO3+	4.662e-05	3.167e-05	-4.331	-4.499	-0.168	
10.45						
NaHCO3	3.702e-05	4.426e-05	-4.432	-4.354	0.078	
1.80						
NaCO3-	1.111e-05	8.361e-06	-4.954	-5.078	-0.123	
4.68						
CaCO3	1.090e-05	1.303e-05	-4.963	-4.885	0.078	-
14.56						
CO2	9.400e-06	1.124e-05	-5.027	-4.949	0.078	
35.16						
MgCO3	9.322e-06	1.115e-05	-5.030	-4.953	0.078	-
17.10						
CO3-2	3.159e-06	6.056e-07	-5.500	-6.218	-0.717	-
1.43						
(CO2)2	3.054e-12	3.652e-12	-11.515	-11.437	0.078	
70.32						
Ca	3.858e-02					
Ca+2	3.728e-02	8.873e-03	-1.429	-2.052	-0.623	-
16.37						
CaSO4	1.246e-03	1.489e-03	-2.905	-2.827	0.078	
7.96						
CaHCO3+	4.662e-05	3.167e-05	-4.331	-4.499	-0.168	
10.45						
CaCO3	1.090e-05	1.303e-05	-4.963	-4.885	0.078	-
14.56						
CaOH+	8.167e-08	6.146e-08	-7.088	-7.211	-0.123	
(0)						
CaHSO4+	3.872e-10	2.914e-10	-9.412	-9.536	-0.123	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.016e-01	-0.185	-0.396	-0.211	
19.13						
H(0)	5.645e-27					
H2	2.823e-27	3.375e-27	-26.549	-26.472	0.078	
28.59						
Mg	5.865e-02					
Mg+2	5.487e-02	1.532e-02	-1.261	-1.815	-0.554	-
20.73						
MgSO4	3.679e-03	4.399e-03	-2.434	-2.357	0.078	
6.30						
MgHCO3+	7.565e-05	4.631e-05	-4.121	-4.334	-0.213	
6.17						
MgOH+	1.217e-05	8.430e-06	-4.915	-5.074	-0.159	
(0)						
MgCO3	9.322e-06	1.115e-05	-5.030	-4.953	0.078	-
17.10						
Na	5.090e-01					

Na+	5.064e-01	3.608e-01	-0.295	-0.443	-0.147
0.10					
NaSO4-	2.537e-03	1.679e-03	-2.596	-2.775	-0.179
21.51					
NaHCO3	3.702e-05	4.426e-05	-4.432	-4.354	0.078
1.80					
NaCO3-	1.111e-05	8.361e-06	-4.954	-5.078	-0.123
4.68					
NaOH	3.688e-17	4.410e-17	-16.433	-16.356	0.078
(0)					
O(0)	2.383e-35				
O2	1.191e-35	1.424e-35	-34.924	-34.846	0.078
31.40					
S(6)	1.260e-02				
SO4-2	5.138e-03	8.480e-04	-2.289	-3.072	-0.782
19.46					
MgSO4	3.679e-03	4.399e-03	-2.434	-2.357	0.078
6.30					
NaSO4-	2.537e-03	1.679e-03	-2.596	-2.775	-0.179
21.51					
CaSO4	1.246e-03	1.489e-03	-2.905	-2.827	0.078
7.96					
HSO4-	3.630e-09	2.731e-09	-8.440	-8.564	-0.123
41.83					
CaHSO4+	3.872e-10	2.914e-10	-9.412	-9.536	-0.123
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.67	-5.12	-4.45	CaSO4
Aragonite	0.18	-8.27	-8.45	CaCO3
Calcite	0.31	-8.27	-8.58	CaCO3
CO2(g)	-3.32	-4.95	-1.63	CO2
Dolomite	1.12	-16.30	-17.42	CaMg(CO3)2
Gypsum	-0.55	-5.14	-4.60	CaSO4:2H2O
H2(g)	-23.34	-26.47	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-31.86	-34.85	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.131 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=20.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=20.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.57
pe 4
redox pe
units mmol/kgw
density 1
Ca 39.80198581
Mg 60.51989303
Na 509
S(6) 12.6
Alkalinity 0.63 as HCO3-
Cl 653
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	6.300e-04	6.300e-04
Ca	3.980e-02	3.980e-02
Cl	6.530e-01	6.530e-01
Mg	6.052e-02	6.052e-02

Na 5.090e-01 5.090e-01
 S(6) 1.260e-02 1.260e-02

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

--

pH = 7.570
 pe = 4.000
 Specific Conductance (µS/cm, 40°C) = 75973
 Density (g/cm³) = 1.01999
 Volume (L) = 1.01880
 Activity of water = 0.978
 Ionic strength (mol/kgw) = 7.817e-01
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 5.962e-04
 Total CO2 (mol/kg) = 5.962e-04
 Temperature (°C) = 40.00
 Electrical balance (eq) = 3.081e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 2.26
 Iterations = 7
 Total H = 1.110130e+02
 Total O = 5.555841e+01

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

--

mole V Species cm³/mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.803e-06	1.064e-06	-5.744	-5.973	-0.229	-
2.01						
H+	3.610e-08	2.692e-08	-7.442	-7.570	-0.128	
0.00						
H2O	5.551e+01	9.784e-01	1.744	-0.009	0.000	
18.16						
C(4)	5.962e-04					
HCO3-	3.792e-04	2.508e-04	-3.421	-3.601	-0.180	
27.93						
MgHCO3+	8.293e-05	5.072e-05	-4.081	-4.295	-0.214	
6.17						
CaHCO3+	5.102e-05	3.464e-05	-4.292	-4.460	-0.168	
10.45						
NaHCO3	3.921e-05	4.694e-05	-4.407	-4.328	0.078	
1.80						
CO2	1.143e-05	1.368e-05	-4.942	-4.864	0.078	
35.16						
CaCO3	1.037e-05	1.241e-05	-4.984	-4.906	0.078	-
14.56						
NaCO3-	1.025e-05	7.723e-06	-4.989	-5.112	-0.123	
4.71						
MgCO3	8.881e-06	1.063e-05	-5.052	-4.973	0.078	-
17.10						
CO3-2	2.924e-06	5.592e-07	-5.534	-6.252	-0.718	-
1.42						

(CO2)2	4.520e-12	5.412e-12	-11.345	-11.267	0.078	
70.32						
Ca	3.980e-02					
Ca+2	3.847e-02	9.154e-03	-1.415	-2.038	-0.624	-
16.37						
CaSO4	1.266e-03	1.516e-03	-2.898	-2.819	0.078	
7.96						
CaHCO3+	5.102e-05	3.464e-05	-4.292	-4.460	-0.168	
10.45						
CaCO3	1.037e-05	1.241e-05	-4.984	-4.906	0.078	-
14.56						
CaOH+	7.331e-08	5.523e-08	-7.135	-7.258	-0.123	
(0)						
CaHSO4+	4.519e-10	3.405e-10	-9.345	-9.468	-0.123	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.013e-01	-0.185	-0.397	-0.211	
19.14						
H(0)	7.432e-27					
H2	3.716e-27	4.449e-27	-26.430	-26.352	0.078	
28.59						
Mg	6.052e-02					
Mg+2	5.667e-02	1.583e-02	-1.247	-1.801	-0.554	-
20.73						
MgSO4	3.744e-03	4.483e-03	-2.427	-2.348	0.078	
6.30						
MgHCO3+	8.293e-05	5.072e-05	-4.081	-4.295	-0.214	
6.17						
MgOH+	1.096e-05	7.585e-06	-4.960	-5.120	-0.160	
(0)						
MgCO3	8.881e-06	1.063e-05	-5.052	-4.973	0.078	-
17.10						
Na	5.090e-01					
Na+	5.064e-01	3.609e-01	-0.295	-0.443	-0.147	
0.11						
NaSO4-	2.505e-03	1.656e-03	-2.601	-2.781	-0.180	
21.55						
NaHCO3	3.921e-05	4.694e-05	-4.407	-4.328	0.078	
1.80						
NaCO3-	1.025e-05	7.723e-06	-4.989	-5.112	-0.123	
4.71						
NaOH	3.209e-17	3.842e-17	-16.494	-16.415	0.078	
(0)						
O(0)	1.369e-35					
O2	6.846e-36	8.196e-36	-35.165	-35.086	0.078	
31.40						
S(6)	1.260e-02					
SO4-2	5.085e-03	8.365e-04	-2.294	-3.078	-0.784	
19.48						
MgSO4	3.744e-03	4.483e-03	-2.427	-2.348	0.078	
6.30						
NaSO4-	2.505e-03	1.656e-03	-2.601	-2.781	-0.180	
21.55						
CaSO4	1.266e-03	1.516e-03	-2.898	-2.819	0.078	
7.96						
HSO4-	4.107e-09	3.094e-09	-8.387	-8.510	-0.123	
41.84						

CaHSO4+ 4.519e-10 3.405e-10 -9.345 -9.468 -0.123
(0)

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

--

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.66	-5.12	-4.45	CaSO4
Aragonite	0.16	-8.29	-8.45	CaCO3
Calcite	0.29	-8.29	-8.58	CaCO3
CO2(g)	-3.24	-4.86	-1.63	CO2
Dolomite	1.08	-16.34	-17.42	CaMg(CO3)2
Gypsum	-0.54	-5.13	-4.60	CaSO4:2H2O
H2(g)	-23.22	-26.35	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-32.10	-35.09	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.138 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=25.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=25.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.55
pe 4
redox pe
units mmol/kgw
density 1
Ca 39.36947855
Mg 59.6673524
Na 509
S(6) 12.6
Alkalinity 0.645 as HCO3-
Cl 653
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	6.450e-04	6.450e-04
Ca	3.937e-02	3.937e-02
Cl	6.530e-01	6.530e-01
Mg	5.967e-02	5.967e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

pH	=	7.550
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	75923
Density (g/cm^3)	=	1.01994
Volume (L)	=	1.01882
Activity of water	=	0.978
Ionic strength (mol/kgw)	=	7.793e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	6.135e-04
Total CO2 (mol/kg)	=	6.135e-04
Temperature (°C)	=	40.00
Electrical balance (eq)	=	2.823e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	2.07
Iterations	=	7
Total H	=	1.110130e+02
Total O	=	5.555846e+01

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

--

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.721e-06	1.017e-06	-5.764	-5.993	-0.229	-
2.01						
H+	3.780e-08	2.818e-08	-7.423	-7.550	-0.127	
0.00						
H2O	5.551e+01	9.785e-01	1.744	-0.009	0.000	
18.16						
C(4)	6.135e-04					
HCO3-	3.921e-04	2.594e-04	-3.407	-3.586	-0.179	
27.93						
MgHCO3+	8.449e-05	5.169e-05	-4.073	-4.287	-0.213	
6.17						
CaHCO3+	5.218e-05	3.544e-05	-4.282	-4.451	-0.168	
10.45						
NaHCO3	4.057e-05	4.855e-05	-4.392	-4.314	0.078	
1.80						
CO2	1.238e-05	1.482e-05	-4.907	-4.829	0.078	
35.16						
CaCO3	1.014e-05	1.213e-05	-4.994	-4.916	0.078	-
14.56						
NaCO3-	1.013e-05	7.628e-06	-4.994	-5.118	-0.123	
4.70						
MgCO3	8.649e-06	1.035e-05	-5.063	-4.985	0.078	-
17.10						
CO3-2	2.885e-06	5.524e-07	-5.540	-6.258	-0.718	-
1.42						
(CO2)2	5.305e-12	6.348e-12	-11.275	-11.197	0.078	
70.32						
Ca	3.937e-02					
Ca+2	3.805e-02	9.054e-03	-1.420	-2.043	-0.623	-
16.37						
CaSO4	1.260e-03	1.508e-03	-2.900	-2.822	0.078	
7.96						
CaHCO3+	5.218e-05	3.544e-05	-4.282	-4.451	-0.168	
10.45						
CaCO3	1.014e-05	1.213e-05	-4.994	-4.916	0.078	-
14.56						
CaOH+	6.928e-08	5.216e-08	-7.159	-7.283	-0.123	
(0)						
CaHSO4+	4.710e-10	3.547e-10	-9.327	-9.450	-0.123	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.014e-01	-0.185	-0.396	-0.211	
19.14						
H(0)	8.154e-27					
H2	4.077e-27	4.878e-27	-26.390	-26.312	0.078	
28.59						
Mg	5.967e-02					
Mg+2	5.585e-02	1.559e-02	-1.253	-1.807	-0.554	-
20.73						

MgSO4	3.713e-03	4.443e-03	-2.430	-2.352	0.078	
6.30						
MgHCO3+	8.449e-05	5.169e-05	-4.073	-4.287	-0.213	
6.17						
MgOH+	1.031e-05	7.138e-06	-4.987	-5.146	-0.160	
(0)						
MgCO3	8.649e-06	1.035e-05	-5.063	-4.985	0.078	-
17.10						
Na	5.090e-01					
Na+	5.064e-01	3.609e-01	-0.295	-0.443	-0.147	
0.11						
NaSO4-	2.519e-03	1.666e-03	-2.599	-2.778	-0.179	
21.54						
NaHCO3	4.057e-05	4.855e-05	-4.392	-4.314	0.078	
1.80						
NaCO3-	1.013e-05	7.628e-06	-4.994	-5.118	-0.123	
4.70						
NaOH	3.066e-17	3.668e-17	-16.513	-16.436	0.078	
(0)						
O(0)	1.139e-35					
O2	5.697e-36	6.817e-36	-35.244	-35.166	0.078	
31.40						
S(6)	1.260e-02					
SO4-2	5.108e-03	8.414e-04	-2.292	-3.075	-0.783	
19.47						
MgSO4	3.713e-03	4.443e-03	-2.430	-2.352	0.078	
6.30						
NaSO4-	2.519e-03	1.666e-03	-2.599	-2.778	-0.179	
21.54						
CaSO4	1.260e-03	1.508e-03	-2.900	-2.822	0.078	
7.96						
HSO4-	4.327e-09	3.258e-09	-8.364	-8.487	-0.123	
41.84						
CaHSO4+	4.710e-10	3.547e-10	-9.327	-9.450	-0.123	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.67	-5.12	-4.45	CaSO4
Aragonite	0.15	-8.30	-8.45	CaCO3
Calcite	0.28	-8.30	-8.58	CaCO3
CO2(g)	-3.20	-4.83	-1.63	CO2
Dolomite	1.06	-16.37	-17.42	CaMg(CO3)2
Gypsum	-0.54	-5.14	-4.60	CaSO4:2H2O
H2(g)	-23.18	-26.31	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-32.18	-35.17	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

Reading input data for simulation 2.

End of Run after 0.136 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=30.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=30.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat
SOLUTION 1
temp 40
pH 7.52
pe 4
redox pe
units mmol/kgw
density 1
Ca 42.79479898
Mg 65.36729068
Na 509
S(6) 12.6
Alkalinity 0.7 as HCO3-
Cl 653
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

--

Elements	Molality	Moles
Alkalinity	7.000e-04	7.000e-04
Ca	4.279e-02	4.279e-02
Cl	6.530e-01	6.530e-01
Mg	6.537e-02	6.537e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

--

pH	=	7.520
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	76284
Density (g/cm^3)	=	1.02037
Volume (L)	=	1.01866
Activity of water	=	0.978
Ionic strength (mol/kgw)	=	7.967e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	6.686e-04
Total CO2 (mol/kg)	=	6.686e-04
Temperature (°C)	=	40.00
Electrical balance (eq)	=	4.642e-02
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	3.37
Iterations	=	7
Total H	=	1.110131e+02
Total O	=	5.555862e+01

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	Gamma
			Molality	Activity		
OH-	1.611e-06	9.485e-07	-5.793	-6.023	-0.230	-
1.99						
H+	4.054e-08	3.020e-08	-7.392	-7.520	-0.128	
0.00						
H2O	5.551e+01	9.783e-01	1.744	-0.010	0.000	
18.16						
C(4)	6.686e-04					
HCO3-	4.184e-04	2.763e-04	-3.378	-3.559	-0.180	
27.97						
MgHCO3+	9.920e-05	6.055e-05	-4.003	-4.218	-0.214	
6.18						
CaHCO3+	6.053e-05	4.104e-05	-4.218	-4.387	-0.169	
10.45						
NaHCO3	4.309e-05	5.176e-05	-4.366	-4.286	0.080	
1.80						
CO2	1.408e-05	1.691e-05	-4.851	-4.772	0.080	
35.16						

CaCO3	1.091e-05	1.311e-05	-4.962	-4.882	0.080	-
14.56						
NaCO3-	1.005e-05	7.591e-06	-4.998	-5.120	-0.122	
4.80						
MgCO3	9.416e-06	1.131e-05	-5.026	-4.946	0.080	-
17.10						
CO3-2	2.889e-06	5.491e-07	-5.539	-6.260	-0.721	-
1.39						
(CO2) 2	6.886e-12	8.273e-12	-11.162	-11.082	0.080	
70.32						
Ca	4.279e-02					
Ca+2	4.141e-02	9.843e-03	-1.383	-2.007	-0.624	-
16.36						
CaSO4	1.311e-03	1.575e-03	-2.882	-2.803	0.080	
7.96						
CaHCO3+	6.053e-05	4.104e-05	-4.218	-4.387	-0.169	
10.45						
CaCO3	1.091e-05	1.311e-05	-4.962	-4.882	0.080	-
14.56						
CaOH+	7.007e-08	5.292e-08	-7.154	-7.276	-0.122	
(0)						
CaHSO4+	5.257e-10	3.970e-10	-9.279	-9.401	-0.122	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.006e-01	-0.185	-0.397	-0.212	
19.14						
H(0)	9.324e-27					
H2	4.662e-27	5.601e-27	-26.331	-26.252	0.080	
28.59						
Mg	6.537e-02					
Mg+2	6.134e-02	1.715e-02	-1.212	-1.766	-0.554	-
20.71						
MgSO4	3.908e-03	4.694e-03	-2.408	-2.328	0.080	
6.30						
MgHCO3+	9.920e-05	6.055e-05	-4.003	-4.218	-0.214	
6.18						
MgOH+	1.059e-05	7.323e-06	-4.975	-5.135	-0.160	
(0)						
MgCO3	9.416e-06	1.131e-05	-5.026	-4.946	0.080	-
17.10						
Na	5.090e-01					
Na+	5.065e-01	3.612e-01	-0.295	-0.442	-0.147	
0.12						
NaSO4-	2.427e-03	1.602e-03	-2.615	-2.795	-0.180	
21.64						
NaHCO3	4.309e-05	5.176e-05	-4.366	-4.286	0.080	
1.80						
NaCO3-	1.005e-05	7.591e-06	-4.998	-5.120	-0.122	
4.80						
NaOH	2.852e-17	3.426e-17	-16.545	-16.465	0.080	
(0)						
O(0)	8.606e-36					
O2	4.303e-36	5.170e-36	-35.366	-35.287	0.080	
31.40						
S(6)	1.260e-02					
SO4-2	4.954e-03	8.085e-04	-2.305	-3.092	-0.787	
19.51						

MgSO4	3.908e-03	4.694e-03	-2.408	-2.328	0.080
6.30					
NaSO4-	2.427e-03	1.602e-03	-2.615	-2.795	-0.180
21.64					
CaSO4	1.311e-03	1.575e-03	-2.882	-2.803	0.080
7.96					
HSO4-	4.442e-09	3.355e-09	-8.352	-8.474	-0.122
41.84					
CaHSO4+	5.257e-10	3.970e-10	-9.279	-9.401	-0.122
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.65	-5.10	-4.45	CaSO4
Aragonite	0.18	-8.27	-8.45	CaCO3
Calcite	0.31	-8.27	-8.58	CaCO3
CO2 (g)	-3.15	-4.77	-1.63	CO2
Dolomite	1.13	-16.29	-17.42	CaMg (CO3) 2
Gypsum	-0.52	-5.12	-4.60	CaSO4:2H2O
H2 (g)	-23.12	-26.25	-3.13	H2
H2O (g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2 (g)	-32.30	-35.29	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.133 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=80.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
1\Appendix\CC\cc_ID=80.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.46
pe 4
redox pe
units mmol/kgw
density 1
Ca 44.23
Mg 67.05
Na 509
S(6) 12.6
Alkalinity 0.62 as HCO3-
Cl 653
water 1 # kgw

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	6.200e-04	6.200e-04
Ca	4.423e-02	4.423e-02
Cl	6.530e-01	6.530e-01
Mg	6.705e-02	6.705e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

pH	=	7.460
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	76411
Density (g/cm^3)	=	1.02052
Volume (L)	=	1.01860
Activity of water	=	0.978
Ionic strength (mol/kgw)	=	8.027e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	5.972e-04
Total CO2 (mol/kg)	=	5.972e-04

Temperature (°C) = 40.00
 Electrical balance (eq) = 5.274e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 3.81
 Iterations = 7
 Total H = 1.110130e+02
 Total O = 5.555841e+01

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

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.404e-06	8.261e-07	-5.853	-6.083	-0.230	-
1.97						
H+	4.656e-08	3.467e-08	-7.332	-7.460	-0.128	
0.00						
H2O	5.551e+01	9.783e-01	1.744	-0.010	0.000	
18.16						
C(4)	5.972e-04					
HCO3-	3.721e-04	2.456e-04	-3.429	-3.610	-0.181	
27.99						
MgHCO3+	9.065e-05	5.528e-05	-4.043	-4.257	-0.215	
6.18						
CaHCO3+	5.565e-05	3.771e-05	-4.255	-4.424	-0.169	
10.45						
NaHCO3	3.826e-05	4.603e-05	-4.417	-4.337	0.080	
1.80						
CO2	1.435e-05	1.726e-05	-4.843	-4.763	0.080	
35.16						
CaCO3	8.720e-06	1.049e-05	-5.059	-4.979	0.080	-
14.56						
NaCO3-	7.775e-06	5.878e-06	-5.109	-5.231	-0.121	
4.83						
MgCO3	7.477e-06	8.995e-06	-5.126	-5.046	0.080	-
17.10						
CO3-2	2.242e-06	4.251e-07	-5.649	-6.372	-0.722	-
1.38						
(CO2)2	7.162e-12	8.616e-12	-11.145	-11.065	0.080	
70.32						
Ca	4.423e-02					
Ca+2	4.283e-02	1.018e-02	-1.368	-1.992	-0.624	-
16.35						
CaSO4	1.337e-03	1.608e-03	-2.874	-2.794	0.080	
7.96						
CaHCO3+	5.565e-05	3.771e-05	-4.255	-4.424	-0.169	
10.45						
CaCO3	8.720e-06	1.049e-05	-5.059	-4.979	0.080	-
14.56						
CaOH+	6.302e-08	4.765e-08	-7.200	-7.322	-0.121	
(0)						
CaHSO4+	6.155e-10	4.653e-10	-9.211	-9.332	-0.121	
(0)						
Cl	6.530e-01					

Cl-	6.530e-01	4.003e-01	-0.185	-0.398	-0.213	
19.15						
H(0)	1.227e-26					
H2	6.137e-27	7.383e-27	-26.212	-26.132	0.080	
28.59						
Mg	6.705e-02					
Mg+2	6.298e-02	1.761e-02	-1.201	-1.754	-0.553	-
20.71						
MgSO4	3.958e-03	4.761e-03	-2.403	-2.322	0.080	
6.30						
MgHCO3+	9.065e-05	5.528e-05	-4.043	-4.257	-0.215	
6.18						
MgOH+	9.479e-06	6.552e-06	-5.023	-5.184	-0.160	
(0)						
MgCO3	7.477e-06	8.995e-06	-5.126	-5.046	0.080	-
17.10						
Na	5.090e-01					
Na+	5.066e-01	3.614e-01	-0.295	-0.442	-0.147	
0.12						
NaSO4-	2.398e-03	1.583e-03	-2.620	-2.801	-0.181	
21.67						
NaHCO3	3.826e-05	4.603e-05	-4.417	-4.337	0.080	
1.80						
NaCO3-	7.775e-06	5.878e-06	-5.109	-5.231	-0.121	
4.83						
NaOH	2.481e-17	2.985e-17	-16.605	-16.525	0.080	
(0)						
O(0)	4.945e-36					
O2	2.473e-36	2.975e-36	-35.607	-35.527	0.080	
31.40						
S(6)	1.260e-02					
SO4-2	4.907e-03	7.983e-04	-2.309	-3.098	-0.789	
19.53						
MgSO4	3.958e-03	4.761e-03	-2.403	-2.322	0.080	
6.30						
NaSO4-	2.398e-03	1.583e-03	-2.620	-2.801	-0.181	
21.67						
CaSO4	1.337e-03	1.608e-03	-2.874	-2.794	0.080	
7.96						
HSO4-	5.030e-09	3.803e-09	-8.298	-8.420	-0.121	
41.85						
CaHSO4+	6.155e-10	4.653e-10	-9.211	-9.332	-0.121	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.64	-5.09	-4.45	CaSO4
Aragonite	0.08	-8.36	-8.45	CaCO3
Calcite	0.22	-8.36	-8.58	CaCO3
CO2(g)	-3.14	-4.76	-1.63	CO2
Dolomite	0.93	-16.49	-17.42	CaMg(CO3)2
Gypsum	-0.51	-5.11	-4.60	CaSO4:2H2O
H2(g)	-23.00	-26.13	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O

Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-32.54	-35.53	-2.98	O2

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.134 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
2\Appendix\sp_ID=80+7.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
2\Appendix\sp_ID=80+7.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

REACTION_PRESSURE 1
6.8
SOLUTION 1
temp 40
pH 7.54
pe 4
redox pe
units mmol/kgw
density 1
Ca 40.86
Mg 61.94
Na 509

S(6) 12.6
 Alkalinity 0.52 as HCO3-
 Cl 653
 water 1 # kgg

 Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	5.200e-04	5.200e-04
Ca	4.086e-02	4.086e-02
Cl	6.530e-01	6.530e-01
Mg	6.194e-02	6.194e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

pH	=	7.540
pe	=	4.000
Specific Conductance (μS/cm, 40°C)	=	76073
Density (g/cm ³)	=	1.02011
Volume (L)	=	1.01875
Activity of water	=	0.978
Ionic strength (mol/kgw)	=	7.865e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	4.926e-04
Total CO2 (mol/kg)	=	4.926e-04
Temperature (°C)	=	40.00
Electrical balance (eq)	=	3.588e-02
Percent error, 100*(Cat- An)/(Cat+ An)	=	2.62
Iterations	=	7
Total H	=	1.110129e+02
Total O	=	5.555810e+01

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

mole V Species cm ³ /mol	Molality	Activity	Log		Log	Gamma
			Molality	Activity		
OH- 2.00	1.684e-06	9.933e-07	-5.774	-6.003	-0.229	-
H+ 0.00	3.869e-08	2.884e-08	-7.412	-7.540	-0.128	
H2O 18.16	5.551e+01	9.784e-01	1.744	-0.009	0.000	
C(4)	4.926e-04					

HCO3-	3.120e-04	2.062e-04	-3.506	-3.686	-0.180	
27.95						
MgHCO3+	6.994e-05	4.275e-05	-4.155	-4.369	-0.214	
6.17						
CaHCO3+	4.311e-05	2.926e-05	-4.365	-4.534	-0.168	
10.45						
NaHCO3	3.222e-05	3.862e-05	-4.492	-4.413	0.079	
1.80						
CO2	1.006e-05	1.206e-05	-4.997	-4.919	0.079	
35.16						
CaCO3	8.164e-06	9.785e-06	-5.088	-5.009	0.079	-
14.56						
NaCO3-	7.865e-06	5.930e-06	-5.104	-5.227	-0.123	
4.74						
MgCO3	6.978e-06	8.363e-06	-5.156	-5.078	0.079	-
17.10						
CO3-2	2.249e-06	4.292e-07	-5.648	-6.367	-0.719	-
1.41						
(CO2) 2	3.507e-12	4.203e-12	-11.455	-11.376	0.079	
70.32						
Ca	4.086e-02					
Ca+2	3.952e-02	9.400e-03	-1.403	-2.027	-0.624	-
16.36						
CaSO4	1.285e-03	1.540e-03	-2.891	-2.813	0.079	
7.96						
CaHCO3+	4.311e-05	2.926e-05	-4.365	-4.534	-0.168	
10.45						
CaCO3	8.164e-06	9.785e-06	-5.088	-5.009	0.079	-
14.56						
CaOH+	7.020e-08	5.293e-08	-7.154	-7.276	-0.123	
(0)						
CaHSO4+	4.916e-10	3.706e-10	-9.308	-9.431	-0.123	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.011e-01	-0.185	-0.397	-0.212	
19.14						
H(0)	8.524e-27					
H2	4.262e-27	5.108e-27	-26.370	-26.292	0.079	
28.59						
Mg	6.194e-02					
Mg+2	5.806e-02	1.622e-02	-1.236	-1.790	-0.554	-
20.72						
MgSO4	3.792e-03	4.545e-03	-2.421	-2.342	0.079	
6.30						
MgHCO3+	6.994e-05	4.275e-05	-4.155	-4.369	-0.214	
6.17						
MgOH+	1.048e-05	7.254e-06	-4.980	-5.139	-0.160	
(0)						
MgCO3	6.978e-06	8.363e-06	-5.156	-5.078	0.079	-
17.10						
Na	5.090e-01					
Na+	5.065e-01	3.610e-01	-0.295	-0.442	-0.147	
0.11						
NaSO4-	2.480e-03	1.639e-03	-2.606	-2.785	-0.180	
21.58						
NaHCO3	3.222e-05	3.862e-05	-4.492	-4.413	0.079	
1.80						

NaCO3-	7.865e-06	5.930e-06	-5.104	-5.227	-0.123
4.74					
NaOH	2.992e-17	3.586e-17	-16.524	-16.445	0.079
(0)					
O(0)	1.037e-35				
O2	5.187e-36	6.216e-36	-35.285	-35.206	0.079
31.40					
S(6)	1.260e-02				
SO4-2	5.043e-03	8.275e-04	-2.297	-3.082	-0.785
19.49					
MgSO4	3.792e-03	4.545e-03	-2.421	-2.342	0.079
6.30					
NaSO4-	2.480e-03	1.639e-03	-2.606	-2.785	-0.180
21.58					
CaSO4	1.285e-03	1.540e-03	-2.891	-2.813	0.079
7.96					
HSO4-	4.350e-09	3.279e-09	-8.362	-8.484	-0.123
41.84					
CaHSO4+	4.916e-10	3.706e-10	-9.308	-9.431	-0.123
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.66	-5.11	-4.45	CaSO4
Aragonite	0.05	-8.39	-8.45	CaCO3
Calcite	0.19	-8.39	-8.58	CaCO3
CO2(g)	-3.29	-4.92	-1.63	CO2
Dolomite	0.87	-16.55	-17.42	CaMg(CO3)2
Gypsum	-0.53	-5.13	-4.60	CaSO4:2H2O
H2(g)	-23.16	-26.29	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-32.22	-35.21	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
C	4.926e-04	4.926e-04
Ca	4.086e-02	4.086e-02
Cl	6.530e-01	6.530e-01

Mg	6.194e-02	6.194e-02
Na	5.090e-01	5.090e-01
S	1.260e-02	1.260e-02

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

--

	pH =	7.538	Charge balance
	pe =	-2.253	Adjusted to redox
equilibrium			
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	76074	
Density (g/cm^3)	=	1.02035	
Volume (L)	=	1.01851	
Activity of water	=	0.978	
Ionic strength (mol/kgw)	=	7.865e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	5.200e-04	
Total CO2 (mol/kg)	=	4.926e-04	
Temperature (°C)	=	40.00	
Pressure (atm)	=	6.80	
Electrical balance (eq)	=	3.588e-02	
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	2.62	
Iterations	=	12	
Total H	=	1.110129e+02	
Total O	=	5.555810e+01	

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

--

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm^3/mol						
OH-	1.684e-06	9.936e-07	-5.774	-6.003	-0.229	-
2.00						
H+	3.886e-08	2.896e-08	-7.411	-7.538	-0.128	
0.00						
H2O	5.551e+01	9.784e-01	1.744	-0.009	0.000	
18.15						
C(-4)	1.401e-25					
CH4	1.401e-25	1.679e-25	-24.854	-24.775	0.079	
36.63						
C(4)	4.926e-04					
HCO3-	3.118e-04	2.061e-04	-3.506	-3.686	-0.180	
27.95						
MgHCO3+	6.995e-05	4.276e-05	-4.155	-4.369	-0.214	
6.19						
CaHCO3+	4.312e-05	2.926e-05	-4.365	-4.534	-0.168	
10.46						
NaHCO3	3.240e-05	3.883e-05	-4.489	-4.411	0.079	
1.80						
CO2	1.004e-05	1.203e-05	-4.998	-4.920	0.079	
35.16						
CaCO3	8.177e-06	9.800e-06	-5.087	-5.009	0.079	-
14.52						

NaCO3-	7.869e-06	5.933e-06	-5.104	-5.227	-0.123	
4.79						
MgCO3	6.986e-06	8.373e-06	-5.156	-5.077	0.079	-
17.05						
CO3-2	2.252e-06	4.300e-07	-5.648	-6.367	-0.719	-
1.36						
(CO2)2	3.494e-12	4.187e-12	-11.457	-11.378	0.079	
70.31						
Ca	4.086e-02					
Ca+2	3.952e-02	9.405e-03	-1.403	-2.027	-0.623	-
16.33						
CaSO4	1.285e-03	1.540e-03	-2.891	-2.813	0.079	
7.98						
CaHCO3+	4.312e-05	2.926e-05	-4.365	-4.534	-0.168	
10.46						
CaCO3	8.177e-06	9.800e-06	-5.087	-5.009	0.079	-
14.52						
CaOH+	6.996e-08	5.275e-08	-7.155	-7.278	-0.123	
(0)						
CaHSO4+	4.946e-10	3.729e-10	-9.306	-9.428	-0.123	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	4.012e-01	-0.185	-0.397	-0.212	
19.14						
H(0)	2.741e-14					
H2	1.371e-14	1.643e-14	-13.863	-13.784	0.079	
28.59						
Mg	6.194e-02					
Mg+2	5.806e-02	1.623e-02	-1.236	-1.790	-0.554	-
20.68						
MgSO4	3.790e-03	4.543e-03	-2.421	-2.343	0.079	
6.32						
MgHCO3+	6.995e-05	4.276e-05	-4.155	-4.369	-0.214	
6.19						
MgOH+	1.044e-05	7.223e-06	-4.982	-5.141	-0.160	
(0)						
MgCO3	6.986e-06	8.373e-06	-5.156	-5.077	0.079	-
17.05						
Na	5.090e-01					
Na+	5.065e-01	3.611e-01	-0.295	-0.442	-0.147	
0.13						
NaSO4-	2.481e-03	1.640e-03	-2.605	-2.785	-0.180	
21.54						
NaHCO3	3.240e-05	3.883e-05	-4.489	-4.411	0.079	
1.80						
NaCO3-	7.869e-06	5.933e-06	-5.104	-5.227	-0.123	
4.79						
NaOH	2.992e-17	3.586e-17	-16.524	-16.445	0.079	
(0)						
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-60.305	-60.226	0.079	
31.39						
S(-2)	8.589e-22					
HS-	7.921e-22	4.673e-22	-21.101	-21.330	-0.229	
21.97						
H2S	6.670e-23	7.994e-23	-22.176	-22.097	0.079	
37.20						

S-2	2.951e-26	5.208e-27	-25.530	-26.283	-0.753
(0)					
S(6)	1.260e-02				
SO4-2	5.044e-03	8.281e-04	-2.297	-3.082	-0.785
19.46					
MgSO4	3.790e-03	4.543e-03	-2.421	-2.343	0.079
6.32					
NaSO4-	2.481e-03	1.640e-03	-2.605	-2.785	-0.180
21.54					
CaSO4	1.285e-03	1.540e-03	-2.891	-2.813	0.079
7.98					
HSO4-	4.349e-09	3.279e-09	-8.362	-8.484	-0.123
41.82					
CaHSO4+	4.946e-10	3.729e-10	-9.306	-9.428	-0.123
(0)					

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

Phase	SI**	log IAP	log K(313 K,	7 atm)
Anhydrite	-0.66	-5.11	-4.45	CaSO4
Aragonite	0.05	-8.39	-8.44	CaCO3
Calcite	0.18	-8.39	-8.57	CaCO3
CH4(g)	-21.86	-24.77	-2.92	CH4
CO2(g)	-3.29	-4.92	-1.63	CO2
Dolomite	0.86	-16.55	-17.41	CaMg(CO3)2
Gypsum	-0.53	-5.13	-4.59	CaSO4:2H2O
H2(g)	-10.65	-13.78	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
H2S(g)	-20.90	-28.87	-7.96	H2S
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-57.24	-60.23	-2.99	O2
Sulfur	-16.07	-11.53	4.54	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

 Reading input data for simulation 2.

 End of Run after 0.152 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
 2\Appendix\sp_ID=80+7+11.pqi
 Output file: D:\KU\Thesis Writing\4) Results\Story
 2\Appendix\sp_ID=80+7+11.pqi
 Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
 15100\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 3.6.2-
15100\database\phreeqc.dat

REACTION_PRESSURE 1

10.89

SOLUTION 1

temp 41
pH 7.49
pe 4
redox pe
units mmol/kgw
density 1
Ca 46.55
Mg 71.22
Na 509
S(6) 12.6
Alkalinity 0.48 as HCO3-
Cl 653
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

--

Elements	Molality	Moles
Alkalinity	4.800e-04	4.800e-04
Ca	4.655e-02	4.655e-02
Cl	6.530e-01	6.530e-01
Mg	7.122e-02	7.122e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

--

pH = 7.490
 pe = 4.000
 Specific Conductance ($\mu\text{S}/\text{cm}$, 41°C) = 77923
 Density (g/cm^3) = 1.02040
 Volume (L) = 1.01890
 Activity of water = 0.978
 Ionic strength (mol/kgw) = $8.150\text{e-}01$
 Mass of water (kg) = $1.000\text{e+}00$
 Total carbon (mol/kg) = $4.541\text{e-}04$
 Total CO_2 (mol/kg) = $4.541\text{e-}04$
 Temperature ($^\circ\text{C}$) = 41.00
 Electrical balance (eq) = $6.586\text{e-}02$
 Percent error, $100 * (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = 4.72
 Iterations = 7
 Total H = $1.110129\text{e+}02$
 Total O = $5.555798\text{e+}01$

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

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	$1.611\text{e-}06$	$9.449\text{e-}07$	-5.793	-6.025	-0.232	-
1.94 H+	$4.350\text{e-}08$	$3.236\text{e-}08$	-7.362	-7.490	-0.128	
0.00 H ₂ O	$5.551\text{e+}01$	$9.782\text{e-}01$	1.744	-0.010	0.000	
18.16 C(4)	$4.541\text{e-}04$					
HCO ₃ -	$2.773\text{e-}04$	$1.827\text{e-}04$	-3.557	-3.738	-0.181	
28.05 MgHCO ₃ +	$7.230\text{e-}05$	$4.398\text{e-}05$	-4.141	-4.357	-0.216	
6.19 CaHCO ₃ +	$4.389\text{e-}05$	$2.969\text{e-}05$	-4.358	-4.527	-0.170	
10.48 NaHCO ₃	$2.823\text{e-}05$	$3.406\text{e-}05$	-4.549	-4.468	0.082	
1.80 CO ₂	$9.889\text{e-}06$	$1.193\text{e-}05$	-5.005	-4.923	0.082	
35.21 CaCO ₃	$7.583\text{e-}06$	$9.149\text{e-}06$	-5.120	-5.039	0.082	-
14.56 NaCO ₃ -	$6.558\text{e-}06$	$4.966\text{e-}06$	-5.183	-5.304	-0.121	
4.96 MgCO ₃	$6.490\text{e-}06$	$7.829\text{e-}06$	-5.188	-5.106	0.082	-
17.10 CO ₃ -2	$1.823\text{e-}06$	$3.431\text{e-}07$	-5.739	-6.465	-0.725	-
1.37 (CO ₂) ₂	$3.506\text{e-}12$	$4.230\text{e-}12$	-11.455	-11.374	0.082	
70.42 Ca	$4.655\text{e-}02$					
Ca+2	$4.514\text{e-}02$	$1.069\text{e-}02$	-1.345	-1.971	-0.626	-
16.33 CaSO ₄	$1.359\text{e-}03$	$1.639\text{e-}03$	-2.867	-2.785	0.082	
7.99						

Anhydrite	-0.62	-5.08	-4.46	CaSO4
Aragonite	0.02	-8.44	-8.45	CaCO3
Calcite	0.15	-8.44	-8.59	CaCO3
CO2(g)	-3.29	-4.92	-1.63	CO2
Dolomite	0.81	-16.63	-17.44	CaMg(CO3)2
Gypsum	-0.51	-5.10	-4.60	CaSO4:2H2O
H2(g)	-23.07	-26.20	-3.13	H2
H2O(g)	-1.12	-0.01	1.12	H2O
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-32.12	-35.11	-2.99	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.

Using pressure 1.

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

--

Elements	Molality	Moles
C	4.541e-04	4.541e-04
Ca	4.655e-02	4.655e-02
Cl	6.530e-01	6.530e-01
Mg	7.122e-02	7.122e-02
Na	5.090e-01	5.090e-01
S	1.260e-02	1.260e-02

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

--

	pH =	7.487	Charge balance
	pe =	9.258	Adjusted to redox
equilibrium			
	Specific Conductance ($\mu\text{S}/\text{cm}$, 41°C)	=	77924
	Density (g/cm^3)	=	1.02082
	Volume (L)	=	1.01848
	Activity of water	=	0.978
	Ionic strength (mol/kgw)	=	8.150e-01
	Mass of water (kg)	=	1.000e+00
	Total alkalinity (eq/kg)	=	4.800e-04
	Total CO2 (mol/kg)	=	4.541e-04
	Temperature (°C)	=	41.00
	Pressure (atm)	=	10.89
	Electrical balance (eq)	=	6.586e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$		=	4.72
	Iterations	=	10
	Total H	=	1.110129e+02
	Total O	=	5.555798e+01

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

--

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.611e-06	9.455e-07	-5.793	-6.024	-0.232	-
1.94						
H+	4.380e-08	3.259e-08	-7.359	-7.487	-0.128	
0.00						
H2O	5.551e+01	9.782e-01	1.744	-0.010	0.000	
18.16						
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-116.671	-116.590	0.082	
36.70						
C(4)	4.541e-04					
HCO3-	2.770e-04	1.825e-04	-3.558	-3.739	-0.181	
28.06						
MgHCO3+	7.232e-05	4.400e-05	-4.141	-4.357	-0.216	
6.22						
CaHCO3+	4.390e-05	2.971e-05	-4.358	-4.527	-0.170	
10.50						
NaHCO3	2.850e-05	3.438e-05	-4.545	-4.464	0.082	
1.80						
CO2	9.854e-06	1.189e-05	-5.006	-4.925	0.082	
35.20						
CaCO3	7.606e-06	9.176e-06	-5.119	-5.037	0.082	-
14.49						
NaCO3-	6.565e-06	4.973e-06	-5.183	-5.303	-0.121	
5.04						
MgCO3	6.505e-06	7.848e-06	-5.187	-5.105	0.082	-
17.02						
CO3-2	1.828e-06	3.443e-07	-5.738	-6.463	-0.725	-
1.29						
(CO2)2	3.481e-12	4.200e-12	-11.458	-11.377	0.082	
70.40						
Ca	4.655e-02					
Ca+2	4.514e-02	1.070e-02	-1.345	-1.971	-0.625	-
16.27						
CaSO4	1.359e-03	1.640e-03	-2.867	-2.785	0.082	
8.01						
CaHCO3+	4.390e-05	2.971e-05	-4.358	-4.527	-0.170	
10.50						
CaCO3	7.606e-06	9.176e-06	-5.119	-5.037	0.082	-
14.49						
CaOH+	7.041e-08	5.333e-08	-7.152	-7.273	-0.121	
(0)						
CaHSO4+	6.011e-10	4.552e-10	-9.221	-9.342	-0.121	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	3.995e-01	-0.185	-0.398	-0.213	
19.16						
H(0)	3.232e-37					

H2	1.616e-37	1.949e-37	-36.792	-36.710	0.082	
28.59						
Mg	7.122e-02					
Mg+2	6.700e-02	1.872e-02	-1.174	-1.728	-0.554	-
20.65						
MgSO4	4.132e-03	4.985e-03	-2.384	-2.302	0.082	
6.35						
MgHCO3+	7.232e-05	4.400e-05	-4.141	-4.357	-0.216	
6.22						
MgOH+	1.163e-05	8.030e-06	-4.934	-5.095	-0.161	
(0)						
MgCO3	6.505e-06	7.848e-06	-5.187	-5.105	0.082	-
17.02						
Na	5.090e-01					
Na+	5.066e-01	3.615e-01	-0.295	-0.442	-0.147	
0.18						
NaSO4-	2.331e-03	1.536e-03	-2.632	-2.814	-0.181	
21.64						
NaHCO3	2.850e-05	3.438e-05	-4.545	-4.464	0.082	
1.80						
NaCO3-	6.565e-06	4.973e-06	-5.183	-5.303	-0.121	
5.04						
NaOH	2.831e-17	3.415e-17	-16.548	-16.467	0.082	
(0)						
O(0)	1.357e-14					
O2	6.783e-15	8.183e-15	-14.169	-14.087	0.082	
31.43						
S(-2)	0.000e+00					
HS-	0.000e+00	0.000e+00	-112.897	-113.128	-0.232	
22.01						
H2S	0.000e+00	0.000e+00	-113.936	-113.854	0.082	
37.20						
S-2	0.000e+00	0.000e+00	-117.344	-118.104	-0.760	
(0)						
S(6)	1.260e-02					
SO4-2	4.777e-03	7.706e-04	-2.321	-3.113	-0.792	
19.60						
MgSO4	4.132e-03	4.985e-03	-2.384	-2.302	0.082	
6.35						
NaSO4-	2.331e-03	1.536e-03	-2.632	-2.814	-0.181	
21.64						
CaSO4	1.359e-03	1.640e-03	-2.867	-2.785	0.082	
8.01						
HSO4-	4.628e-09	3.505e-09	-8.335	-8.455	-0.121	
41.86						
CaHSO4+	6.011e-10	4.552e-10	-9.221	-9.342	-0.121	
(0)						

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

Phase	SI**	log IAP	log K(314 K, 11 atm)	
Anhydrite	-0.63	-5.08	-4.46	CaSO4
Aragonite	0.01	-8.43	-8.45	CaCO3
Calcite	0.14	-8.43	-8.58	CaCO3
CH4(g)	-113.67	-116.59	-2.92	CH4

CO2(g)	-3.28	-4.92	-1.64	CO2
Dolomite	0.80	-16.62	-17.42	CaMg(CO3)2
Gypsum	-0.51	-5.10	-4.59	CaSO4:2H2O
H2(g)	-33.58	-36.71	-3.13	H2
H2O(g)	-1.12	-0.01	1.11	H2O
H2S(g)	-112.65	-120.62	-7.96	H2S
Halite	-2.42	-0.84	1.58	NaCl
O2(g)	-11.09	-14.09	-2.99	O2
Sulfur	-84.89	-80.36	4.52	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.158 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
2\Appendix\sp_ID=80+7+11+7.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
2\Appendix\sp_ID=80+7+11+7.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat
REACTION_PRESSURE 1
61.24
SOLUTION 1
temp 47
pH 7.85

```

pe          4
redox      pe
units      mmol/kgw
density    1
Ca         43.23
Mg         66.49
Na         509
S(6)      12.6
Alkalinity 0.42 as HCO3-
Cl         653
water     1 # kgg

```

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	4.200e-04	4.200e-04
Ca	4.323e-02	4.323e-02
Cl	6.530e-01	6.530e-01
Mg	6.649e-02	6.649e-02
Na	5.090e-01	5.090e-01
S(6)	1.260e-02	1.260e-02

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

```

pH = 7.850
pe = 4.000
Specific Conductance (µS/cm, 47°C) = 85194
Density (g/cm³) = 1.01742
Volume (L) = 1.02164
Activity of water = 0.978
Ionic strength (mol/kgw) = 7.987e-01
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 3.349e-04
Total CO2 (mol/kg) = 3.349e-04
Temperature (°C) = 47.00
Electrical balance (eq) = 4.982e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 3.61
Iterations = 6
Total H = 1.110128e+02
Total O = 5.555766e+01

```

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

mole V Species cm ³ /mol	Molality	Activity	Log		Gamma
			Molality	Activity	

OH-	5.406e-06	3.162e-06	-5.267	-5.500	-0.233	-
1.91						
H+	1.903e-08	1.413e-08	-7.721	-7.850	-0.129	
0.00						
H2O	5.551e+01	9.783e-01	1.744	-0.010	0.000	
18.21						
C(4)	3.349e-04					
HCO3-	1.930e-04	1.268e-04	-3.715	-3.897	-0.182	
28.14						
MgHCO3+	4.808e-05	2.917e-05	-4.318	-4.535	-0.217	
6.27						
CaHCO3+	2.905e-05	1.961e-05	-4.537	-4.708	-0.171	
10.61						
NaHCO3	1.898e-05	2.281e-05	-4.722	-4.642	0.080	
1.80						
NaCO3-	1.459e-05	1.098e-05	-4.836	-4.960	-0.123	
5.14						
CaCO3	1.411e-05	1.695e-05	-4.851	-4.771	0.080	-
14.54						
MgCO3	1.108e-05	1.331e-05	-4.956	-4.876	0.080	-
17.10						
CO3-2	3.133e-06	5.838e-07	-5.504	-6.234	-0.730	-
1.63						
CO2	2.952e-06	3.548e-06	-5.530	-5.450	0.080	
35.51						
(CO2)2	3.648e-13	4.385e-13	-12.438	-12.358	0.080	
71.02						
Ca	4.323e-02					
Ca+2	4.192e-02	9.762e-03	-1.378	-2.010	-0.633	-
16.31						
CaSO4	1.271e-03	1.527e-03	-2.896	-2.816	0.080	
8.13						
CaHCO3+	2.905e-05	1.961e-05	-4.537	-4.708	-0.171	
10.61						
CaCO3	1.411e-05	1.695e-05	-4.851	-4.771	0.080	-
14.54						
CaOH+	1.491e-07	1.122e-07	-6.827	-6.950	-0.123	
(0)						
CaHSO4+	2.715e-10	2.043e-10	-9.566	-9.690	-0.123	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	3.980e-01	-0.185	-0.400	-0.215	
19.17						
H(0)	1.917e-27					
H2	9.584e-28	1.152e-27	-27.018	-26.939	0.080	
28.59						
Mg	6.649e-02					
Mg+2	6.214e-02	1.705e-02	-1.207	-1.768	-0.562	-
20.90						
MgSO4	4.252e-03	5.110e-03	-2.371	-2.292	0.080	
6.47						
MgHCO3+	4.808e-05	2.917e-05	-4.318	-4.535	-0.217	
6.27						
MgOH+	3.960e-05	2.726e-05	-4.402	-4.564	-0.162	
(0)						
MgCO3	1.108e-05	1.331e-05	-4.956	-4.876	0.080	-
17.10						

Na	5.090e-01					
Na+	5.066e-01	3.593e-01	-0.295	-0.445	-0.149	
0.31						
NaSO4-	2.355e-03	1.547e-03	-2.628	-2.811	-0.182	
21.38						
NaHCO3	1.898e-05	2.281e-05	-4.722	-4.642	0.080	
1.80						
NaCO3-	1.459e-05	1.098e-05	-4.836	-4.960	-0.123	
5.14						
NaOH	9.452e-17	1.136e-16	-16.024	-15.945	0.080	
(0)						
O(0)	2.048e-32					
O2	1.024e-32	1.231e-32	-31.990	-31.910	0.080	
31.77						
S(6)	1.260e-02					
SO4-2	4.723e-03	7.545e-04	-2.326	-3.122	-0.797	
20.01						
MgSO4	4.252e-03	5.110e-03	-2.371	-2.292	0.080	
6.47						
NaSO4-	2.355e-03	1.547e-03	-2.628	-2.811	-0.182	
21.38						
CaSO4	1.271e-03	1.527e-03	-2.896	-2.816	0.080	
8.13						
HSO4-	2.313e-09	1.741e-09	-8.636	-8.759	-0.123	
42.09						
CaHSO4+	2.715e-10	2.043e-10	-9.566	-9.690	-0.123	
(0)						

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

Phase	SI**	log IAP	log K(320 K,	1 atm)
Anhydrite	-0.59	-5.13	-4.54	CaSO4
Aragonite	0.26	-8.24	-8.51	CaCO3
Calcite	0.39	-8.24	-8.64	CaCO3
CO2(g)	-3.76	-5.45	-1.69	CO2
Dolomite	1.32	-16.25	-17.57	CaMg(CO3)2
Gypsum	-0.54	-5.15	-4.61	CaSO4:2H2O
H2(g)	-23.80	-26.94	-3.13	H2
H2O(g)	-0.99	-0.01	0.98	H2O
Halite	-2.43	-0.84	1.59	NaCl
O2(g)	-28.89	-31.91	-3.02	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

--

Elements	Molality	Moles
C	3.349e-04	3.349e-04
Ca	4.323e-02	4.323e-02
Cl	6.530e-01	6.530e-01
Mg	6.649e-02	6.649e-02
Na	5.090e-01	5.090e-01
S	1.260e-02	1.260e-02

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

--

	pH =	7.837	Charge balance
	pe =	-2.520	Adjusted to redox
equilibrium			
	Specific Conductance ($\mu\text{S}/\text{cm}$, 47°C)	= 85142	
	Density (g/cm^3)	= 1.01994	
	Volume (L)	= 1.01912	
	Activity of water	= 0.978	
	Ionic strength (mol/kgw)	= 7.988e-01	
	Mass of water (kg)	= 1.000e+00	
	Total alkalinity (eq/kg)	= 4.200e-04	
	Total CO2 (mol/kg)	= 3.349e-04	
	Temperature (°C)	= 47.00	
	Pressure (atm)	= 61.24	
	Electrical balance (eq)	= 4.982e-02	
	Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	= 3.61	
	Iterations	= 13	
	Total H	= 1.110128e+02	
	Total O	= 5.555766e+01	

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	Gamma
			Molality	Activity		
OH-	5.490e-06	3.216e-06	-5.260	-5.493	-0.232	-
1.97 H+	1.957e-08	1.454e-08	-7.708	-7.837	-0.129	
0.00 H2O	5.551e+01	9.783e-01	1.744	-0.010	0.000	
18.16 C(-4)	2.628e-27					
CH4	2.628e-27	3.159e-27	-26.580	-26.500	0.080	
37.16 C(4)	3.349e-04					
HCO3-	1.911e-04	1.257e-04	-3.719	-3.901	-0.182	
28.20 MgHCO3+	4.802e-05	2.917e-05	-4.319	-4.535	-0.216	
6.45						

CaHCO3+	2.903e-05	1.962e-05	-4.537	-4.707	-0.170	
10.73						
NaHCO3	2.004e-05	2.409e-05	-4.698	-4.618	0.080	
1.80						
NaCO3-	1.482e-05	1.116e-05	-4.829	-4.952	-0.123	
5.65						
CaCO3	1.451e-05	1.744e-05	-4.838	-4.758	0.080	-
14.14						
MgCO3	1.134e-05	1.364e-05	-4.945	-4.865	0.080	-
16.66						
CO3-2	3.211e-06	6.014e-07	-5.493	-6.221	-0.727	-
1.15						
CO2	2.844e-06	3.418e-06	-5.546	-5.466	0.080	
35.45						
(CO2) 2	3.385e-13	4.068e-13	-12.470	-12.391	0.080	
70.89						
Ca	4.323e-02					
Ca+2	4.191e-02	9.815e-03	-1.378	-2.008	-0.630	-
15.91						
CaSO4	1.273e-03	1.530e-03	-2.895	-2.815	0.080	
8.27						
CaHCO3+	2.903e-05	1.962e-05	-4.537	-4.707	-0.170	
10.73						
CaCO3	1.451e-05	1.744e-05	-4.838	-4.758	0.080	-
14.14						
CaOH+	1.462e-07	1.101e-07	-6.835	-6.958	-0.123	
(0)						
CaHSO4+	2.852e-10	2.148e-10	-9.545	-9.668	-0.123	
(0)						
Cl	6.530e-01					
Cl-	6.530e-01	3.987e-01	-0.185	-0.399	-0.214	
19.18						
H(0)	2.088e-14					
H2	1.044e-14	1.255e-14	-13.981	-13.901	0.080	
28.56						
Mg	6.649e-02					
Mg+2	6.216e-02	1.714e-02	-1.206	-1.766	-0.560	-
20.45						
MgSO4	4.232e-03	5.086e-03	-2.373	-2.294	0.080	
6.61						
MgHCO3+	4.802e-05	2.917e-05	-4.319	-4.535	-0.216	
6.45						
MgOH+	3.842e-05	2.648e-05	-4.415	-4.577	-0.162	
(0)						
MgCO3	1.134e-05	1.364e-05	-4.945	-4.865	0.080	-
16.66						
Na	5.090e-01					
Na+	5.066e-01	3.598e-01	-0.295	-0.444	-0.149	
0.49						
NaSO4-	2.367e-03	1.557e-03	-2.626	-2.808	-0.182	
20.99						
NaHCO3	2.004e-05	2.409e-05	-4.698	-4.618	0.080	
1.80						
NaCO3-	1.482e-05	1.116e-05	-4.829	-4.952	-0.123	
5.65						
NaOH	9.596e-17	1.153e-16	-16.018	-15.938	0.080	
(0)						

O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-58.116	-58.036	0.080	
31.64						
S(-2)	2.173e-23					
HS-	2.099e-23	1.230e-23	-22.678	-22.910	-0.232	
22.11						
H2S	7.387e-25	8.879e-25	-24.132	-24.052	0.080	
37.12						
S-2	2.528e-27	4.371e-28	-26.597	-27.359	-0.762	
(0)						
S(6)	1.260e-02					
SO4-2	4.728e-03	7.594e-04	-2.325	-3.120	-0.794	
19.79						
MgSO4	4.232e-03	5.086e-03	-2.373	-2.294	0.080	
6.61						
NaSO4-	2.367e-03	1.557e-03	-2.626	-2.808	-0.182	
20.99						
CaSO4	1.273e-03	1.530e-03	-2.895	-2.815	0.080	
8.27						
HSO4-	2.277e-09	1.715e-09	-8.643	-8.766	-0.123	
41.92						
CaHSO4+	2.852e-10	2.148e-10	-9.545	-9.668	-0.123	
(0)						

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

Phase	SI**	log IAP	log K(320 K,	61 atm)
Anhydrite	-0.63	-5.13	-4.50	CaSO4
Aragonite	0.23	-8.23	-8.46	CaCO3
Calcite	0.35	-8.23	-8.58	CaCO3
CH4(g)	-23.52	-26.50	-2.98	CH4
CO2(g)	-3.74	-5.47	-1.72	CO2
Dolomite	1.25	-16.22	-17.46	CaMg(CO3)2
Gypsum	-0.57	-5.15	-4.58	CaSO4:2H2O
H2(g)	-10.74	-13.90	-3.16	H2
H2O(g)	-0.97	-0.01	0.96	H2O
H2S(g)	-22.77	-30.75	-7.97	H2S
Halite	-2.44	-0.84	1.59	NaCl
O2(g)	-54.99	-58.04	-3.05	O2
Sulfur	-17.78	-13.42	4.37	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.158 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
3\May10\phreeqc\May10_ID=0.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
3\May10\phreeqc\May10_ID=0.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 38.62
Mg 55.18
Na 445
S(6) 11
Alkalinity 1 as HCO3-
Cl 572
water 1 # kgw

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	1.000e-03	1.000e-03
Ca	3.862e-02	3.862e-02
Cl	5.720e-01	5.720e-01
Mg	5.518e-02	5.518e-02

Na 4.450e-01 4.450e-01
 S(6) 1.100e-02 1.100e-02

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

--

pH = 8.200
 pe = 4.000
 Specific Conductance (µS/cm, 40°C) = 68291
 Density (g/cm³) = 1.01693
 Volume (L) = 1.01728
 Activity of water = 0.981
 Ionic strength (mol/kgw) = 6.960e-01
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 7.976e-04
 Total CO2 (mol/kg) = 7.976e-04
 Temperature (°C) = 40.00
 Electrical balance (eq) = 3.760e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 3.12
 Iterations = 6
 Total H = 1.110131e+02
 Total O = 5.555266e+01

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

--

mole V Species cm³/mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	7.597e-06	4.553e-06	-5.119	-5.342	-0.222	-
2.16						
H+	8.423e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00						
H2O	5.551e+01	9.810e-01	1.744	-0.008	0.000	
18.16						
C(4)	7.976e-04					
HCO3-	4.491e-04	2.998e-04	-3.348	-3.523	-0.176	
27.71						
MgHCO3+	8.908e-05	5.521e-05	-4.050	-4.258	-0.208	
6.16						
CaHCO3+	5.918e-05	4.051e-05	-4.228	-4.392	-0.165	
10.44						
CaCO3	5.276e-05	6.193e-05	-4.278	-4.208	0.070	-
14.56						
NaCO3-	4.619e-05	3.433e-05	-4.335	-4.464	-0.129	
4.22						
MgCO3	4.206e-05	4.937e-05	-4.376	-4.307	0.070	-
17.10						
NaHCO3	4.167e-05	4.891e-05	-4.380	-4.311	0.070	
1.80						
CO3-2	1.436e-05	2.852e-06	-4.843	-5.545	-0.702	-
1.61						
CO2	3.257e-06	3.824e-06	-5.487	-5.418	0.070	
35.16						

(CO2)2	3.601e-13	4.227e-13	-12.444	-12.374	0.070	
70.32						
Ca	3.862e-02					
Ca+2	3.732e-02	8.956e-03	-1.428	-2.048	-0.620	-
16.44						
CaSO4	1.183e-03	1.389e-03	-2.927	-2.857	0.070	
7.96						
CaHCO3+	5.918e-05	4.051e-05	-4.228	-4.392	-0.165	
10.44						
CaCO3	5.276e-05	6.193e-05	-4.278	-4.208	0.070	-
14.56						
CaOH+	3.110e-07	2.311e-07	-6.507	-6.636	-0.129	
(0)						
CaHSO4+	9.841e-11	7.313e-11	-10.007	-10.136	-0.129	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.555e-01	-0.243	-0.449	-0.207	
19.09						
H(0)	4.165e-28					
H2	2.083e-28	2.445e-28	-27.681	-27.612	0.070	
28.59						
Mg	5.518e-02					
Mg+2	5.175e-02	1.441e-02	-1.286	-1.841	-0.555	-
20.79						
MgSO4	3.257e-03	3.823e-03	-2.487	-2.418	0.070	
6.30						
MgHCO3+	8.908e-05	5.521e-05	-4.050	-4.258	-0.208	
6.16						
MgOH+	4.235e-05	2.954e-05	-4.373	-4.530	-0.156	
(0)						
MgCO3	4.206e-05	4.937e-05	-4.376	-4.307	0.070	-
17.10						
Na	4.450e-01					
Na+	4.429e-01	3.146e-01	-0.354	-0.502	-0.149	
0.06						
NaSO4-	2.026e-03	1.352e-03	-2.693	-2.869	-0.176	
21.03						
NaCO3-	4.619e-05	3.433e-05	-4.335	-4.464	-0.129	
4.22						
NaHCO3	4.167e-05	4.891e-05	-4.380	-4.311	0.070	
1.80						
NaOH	1.220e-16	1.432e-16	-15.914	-15.844	0.070	
(0)						
O(0)	4.648e-33					
O2	2.324e-33	2.728e-33	-32.634	-32.564	0.070	
31.40						
S(6)	1.100e-02					
SO4-2	4.535e-03	7.834e-04	-2.343	-3.106	-0.763	
19.26						
MgSO4	3.257e-03	3.823e-03	-2.487	-2.418	0.070	
6.30						
NaSO4-	2.026e-03	1.352e-03	-2.693	-2.869	-0.176	
21.03						
CaSO4	1.183e-03	1.389e-03	-2.927	-2.857	0.070	
7.96						
HSO4-	9.139e-10	6.792e-10	-9.039	-9.168	-0.129	
41.79						

CaHSO4+ 9.841e-11 7.313e-11 -10.007 -10.136 -0.129
(0)

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.70	-5.15	-4.45	CaSO4
Aragonite	0.85	-7.59	-8.45	CaCO3
Calcite	0.99	-7.59	-8.58	CaCO3
CO2(g)	-3.79	-5.42	-1.63	CO2
Dolomite	2.44	-14.98	-17.42	CaMg(CO3)2
Gypsum	-0.57	-5.17	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-29.58	-32.56	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.156 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
3\May10_CC\phreeqc\May10_ID=0_theory.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
3\May10_CC\phreeqc\May10_ID=0_theory.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 37.84
Mg 51.89
Na 445
S(6) 11
Alkalinity 2.59 as HCO3-
Cl 572
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.590e-03	2.590e-03
Ca	3.784e-02	3.784e-02
Cl	5.720e-01	5.720e-01
Mg	5.189e-02	5.189e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	68129
Density (g/cm^3)	=	1.01680
Volume (L)	=	1.01738
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.881e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	2.139e-03
Total CO2 (mol/kg)	=	2.139e-03
Temperature (°C)	=	40.00
Electrical balance (eq)	=	2.787e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	2.33
Iterations	=	7
Total H	=	1.110142e+02
Total O	=	5.555667e+01

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

--

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	7.586e-06	4.553e-06	-5.120	-5.342	-0.222	-
2.17						
H+	8.419e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00						
H2O	5.551e+01	9.811e-01	1.744	-0.008	0.000	
18.16						
C(4)	2.139e-03					
HCO3-	1.221e-03	8.159e-04	-2.913	-3.088	-0.175	
27.69						
MgHCO3+	2.264e-04	1.405e-04	-3.645	-3.852	-0.207	
6.16						
CaHCO3+	1.570e-04	1.075e-04	-3.804	-3.968	-0.164	
10.44						
CaCO3	1.403e-04	1.644e-04	-3.853	-3.784	0.069	-
14.56						
NaCO3-	1.258e-04	9.337e-05	-3.900	-4.030	-0.129	
4.18						
NaHCO3	1.135e-04	1.330e-04	-3.945	-3.876	0.069	
1.80						
MgCO3	1.072e-04	1.256e-04	-3.970	-3.901	0.069	-
17.10						
CO3-2	3.895e-05	7.761e-06	-4.410	-5.110	-0.701	-
1.63						
CO2	8.882e-06	1.041e-05	-5.052	-4.983	0.069	
35.16						
(CO2)2	2.672e-12	3.131e-12	-11.573	-11.504	0.069	
70.32						
Ca	3.784e-02					
Ca+2	3.636e-02	8.734e-03	-1.439	-2.059	-0.619	-
16.45						
CaSO4	1.184e-03	1.387e-03	-2.927	-2.858	0.069	
7.96						
CaHCO3+	1.570e-04	1.075e-04	-3.804	-3.968	-0.164	
10.44						
CaCO3	1.403e-04	1.644e-04	-3.853	-3.784	0.069	-
14.56						
CaOH+	3.036e-07	2.254e-07	-6.518	-6.647	-0.129	
(0)						
CaHSO4+	9.838e-11	7.302e-11	-10.007	-10.137	-0.129	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.559e-01	-0.243	-0.449	-0.206	
19.09						
H(0)	4.173e-28					
H2	2.087e-28	2.445e-28	-27.681	-27.612	0.069	
28.59						
Mg	5.189e-02					
Mg+2	4.839e-02	1.347e-02	-1.315	-1.870	-0.555	-
20.80						

MgSO4	3.124e-03	3.661e-03	-2.505	-2.436	0.069	
6.30						
MgHCO3+	2.264e-04	1.405e-04	-3.645	-3.852	-0.207	
6.16						
MgCO3	1.072e-04	1.256e-04	-3.970	-3.901	0.069	-
17.10						
MgOH+	3.958e-05	2.763e-05	-4.403	-4.559	-0.156	
(0)						
Na	4.450e-01					
Na+	4.427e-01	3.144e-01	-0.354	-0.503	-0.149	
0.06						
NaSO4-	2.071e-03	1.384e-03	-2.684	-2.859	-0.175	
20.98						
NaCO3-	1.258e-04	9.337e-05	-3.900	-4.030	-0.129	
4.18						
NaHCO3	1.135e-04	1.330e-04	-3.945	-3.876	0.069	
1.80						
NaOH	1.222e-16	1.431e-16	-15.913	-15.844	0.069	
(0)						
O(0)	4.657e-33					
O2	2.329e-33	2.728e-33	-32.633	-32.564	0.069	
31.40						
S(6)	1.100e-02					
SO4-2	4.621e-03	8.022e-04	-2.335	-3.096	-0.760	
19.24						
MgSO4	3.124e-03	3.661e-03	-2.505	-2.436	0.069	
6.30						
NaSO4-	2.071e-03	1.384e-03	-2.684	-2.859	-0.175	
20.98						
CaSO4	1.184e-03	1.387e-03	-2.927	-2.858	0.069	
7.96						
HSO4-	9.370e-10	6.955e-10	-9.028	-9.158	-0.129	
41.79						
CaHSO4+	9.838e-11	7.302e-11	-10.007	-10.137	-0.129	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.70	-5.15	-4.45	CaSO4
Aragonite	1.28	-7.17	-8.45	CaCO3
Calcite	1.41	-7.17	-8.58	CaCO3
CO2(g)	-3.36	-4.98	-1.63	CO2
Dolomite	3.27	-14.15	-17.42	CaMg(CO3)2
Gypsum	-0.57	-5.17	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-29.58	-32.56	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

Reading input data for simulation 2.

End of Run after 0.028 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
3\May10\phreeqc\May10_ID=14.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
3\May10\phreeqc\May10_ID=14.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.7
pe 4
redox pe
units mmol/kgw
density 1
Ca 37.03
Mg 53.79
Na 445
S(6) 11
Alkalinity 0.6 as HCO3-
Cl 572
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

--

Elements	Molality	Moles
Alkalinity	6.000e-04	6.000e-04
Ca	3.703e-02	3.703e-02
Cl	5.720e-01	5.720e-01
Mg	5.379e-02	5.379e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

--

pH	=	7.700
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	68156
Density (g/cm^3)	=	1.01677
Volume (L)	=	1.01733
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.905e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	5.542e-04
Total CO2 (mol/kg)	=	5.542e-04
Temperature (°C)	=	40.00
Electrical balance (eq)	=	3.204e-02
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	2.67
Iterations	=	6
Total H	=	1.110130e+02
Total O	=	5.555189e+01

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	2.400e-06	1.440e-06	-5.620	-5.842	-0.222	-
2.17						
H+	2.663e-08	1.995e-08	-7.575	-7.700	-0.125	
0.00						
H2O	5.551e+01	9.811e-01	1.744	-0.008	0.000	
18.16						
C(4)	5.542e-04					
HCO3-	3.591e-04	2.398e-04	-3.445	-3.620	-0.175	
27.69						
MgHCO3+	6.946e-05	4.309e-05	-4.158	-4.366	-0.207	
6.16						
CaHCO3+	4.545e-05	3.113e-05	-4.342	-4.507	-0.164	
10.44						
NaHCO3	3.338e-05	3.913e-05	-4.477	-4.407	0.069	
1.80						
CaCO3	1.284e-05	1.505e-05	-4.892	-4.822	0.069	-
14.56						

NaCO3-	1.170e-05	8.685e-06	-4.932	-5.061	-0.129	
4.19						
MgCO3	1.039e-05	1.218e-05	-4.983	-4.914	0.069	-
17.10						
CO2	8.252e-06	9.674e-06	-5.083	-5.014	0.069	
35.16						
CO3-2	3.625e-06	7.215e-07	-5.441	-6.142	-0.701	-
1.62						
(CO2) 2	2.308e-12	2.706e-12	-11.637	-11.568	0.069	
70.32						
Ca	3.703e-02					
Ca+2	3.582e-02	8.601e-03	-1.446	-2.065	-0.620	-
16.45						
CaSO4	1.152e-03	1.351e-03	-2.939	-2.869	0.069	
7.96						
CaHCO3+	4.545e-05	3.113e-05	-4.342	-4.507	-0.164	
10.44						
CaCO3	1.284e-05	1.505e-05	-4.892	-4.822	0.069	-
14.56						
CaOH+	9.453e-08	7.019e-08	-7.024	-7.154	-0.129	
(0)						
CaHSO4+	3.029e-10	2.249e-10	-9.519	-9.648	-0.129	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.558e-01	-0.243	-0.449	-0.206	
19.09						
H(0)	4.171e-27					
H2	2.085e-27	2.445e-27	-26.681	-26.612	0.069	
28.59						
Mg	5.379e-02					
Mg+2	5.048e-02	1.406e-02	-1.297	-1.852	-0.555	-
20.80						
MgSO4	3.221e-03	3.776e-03	-2.492	-2.423	0.069	
6.30						
MgHCO3+	6.946e-05	4.309e-05	-4.158	-4.366	-0.207	
6.16						
MgOH+	1.306e-05	9.112e-06	-4.884	-5.040	-0.156	
(0)						
MgCO3	1.039e-05	1.218e-05	-4.983	-4.914	0.069	-
17.10						
Na	4.450e-01					
Na+	4.429e-01	3.146e-01	-0.354	-0.502	-0.149	
0.06						
NaSO4-	2.050e-03	1.369e-03	-2.688	-2.864	-0.175	
20.99						
NaHCO3	3.338e-05	3.913e-05	-4.477	-4.407	0.069	
1.80						
NaCO3-	1.170e-05	8.685e-06	-4.932	-5.061	-0.129	
4.19						
NaOH	3.863e-17	4.529e-17	-16.413	-16.344	0.069	
(0)						
O(0)	4.655e-35					
O2	2.327e-35	2.728e-35	-34.633	-34.564	0.069	
31.40						
S(6)	1.100e-02					
SO4-2	4.577e-03	7.933e-04	-2.339	-3.101	-0.761	
19.25						

MgSO4	3.221e-03	3.776e-03	-2.492	-2.423	0.069
6.30					
NaSO4-	2.050e-03	1.369e-03	-2.688	-2.864	-0.175
20.99					
CaSO4	1.152e-03	1.351e-03	-2.939	-2.869	0.069
7.96					
HSO4-	2.929e-09	2.175e-09	-8.533	-8.663	-0.129
41.79					
CaHSO4+	3.029e-10	2.249e-10	-9.519	-9.648	-0.129
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.71	-5.17	-4.45	CaSO4
Aragonite	0.24	-8.21	-8.45	CaCO3
Calcite	0.37	-8.21	-8.58	CaCO3
CO2 (g)	-3.39	-5.01	-1.63	CO2
Dolomite	1.22	-16.20	-17.42	CaMg (CO3) 2
Gypsum	-0.59	-5.18	-4.60	CaSO4:2H2O
H2 (g)	-23.48	-26.61	-3.13	H2
H2O (g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2 (g)	-31.58	-34.56	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.164 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
3\May10\phreeqc\May10_ID=14+7.pqi

Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
3\May10\phreeqc\May10_ID=14+7.pqo

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.69
pe 4
redox pe
units mmol/kgw
density 1
Ca 33.12
Mg 48.07
Na 445
S(6) 11
Alkalinity 0.52 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
11

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	5.200e-04	5.200e-04
Ca	3.312e-02	3.312e-02
Cl	5.720e-01	5.720e-01
Mg	4.807e-02	4.807e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	7.690
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67730
Density (g/cm^3)	=	1.01631
Volume (L)	=	1.01749
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.721e-01
Mass of water (kg)	=	1.000e+00

Total carbon (mol/kg) = 4.822e-04
 Total CO2 (mol/kg) = 4.822e-04
 Temperature (°C) = 40.00
 Electrical balance (eq) = 1.286e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.09
 Iterations = 6
 Total H = 1.110129e+02
 Total O = 5.555167e+01

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

mole V			Log	Log	Log		
Species	Molality	Activity	Molality	Activity	Gamma		
cm ³ /mol							
2.20	OH-	2.337e-06	1.407e-06	-5.631	-5.852	-0.220	-
0.00	H+	2.722e-08	2.042e-08	-7.565	-7.690	-0.125	
18.16	H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
C(4)		4.822e-04					
27.65	HCO3-	3.212e-04	2.150e-04	-3.493	-3.668	-0.174	
6.16	MgHCO3+	5.531e-05	3.442e-05	-4.257	-4.463	-0.206	
10.44	CaHCO3+	3.641e-05	2.499e-05	-4.439	-4.602	-0.164	
1.80	NaHCO3	3.003e-05	3.505e-05	-4.522	-4.455	0.067	
4.09	NaCO3-	1.027e-05	7.603e-06	-4.989	-5.119	-0.130	
14.56	CaCO3	1.011e-05	1.180e-05	-4.995	-4.928	0.067	-
17.10	MgCO3	8.147e-06	9.510e-06	-5.089	-5.022	0.067	-
35.16	CO2	7.600e-06	8.873e-06	-5.119	-5.052	0.067	
1.67	CO3-2	3.147e-06	6.320e-07	-5.502	-6.199	-0.697	-
70.32	(CO2)2	1.950e-12	2.276e-12	-11.710	-11.643	0.067	
Ca		3.312e-02					
16.46	Ca+2	3.199e-02	7.701e-03	-1.495	-2.113	-0.618	-
7.96	CaSO4	1.086e-03	1.268e-03	-2.964	-2.897	0.067	
10.44	CaHCO3+	3.641e-05	2.499e-05	-4.439	-4.602	-0.164	
14.56	CaCO3	1.011e-05	1.180e-05	-4.995	-4.928	0.067	-
(0)	CaOH+	8.294e-08	6.142e-08	-7.081	-7.212	-0.130	
(0)	CaHSO4+	2.918e-10	2.161e-10	-9.535	-9.665	-0.130	

Cl	5.720e-01					
Cl-	5.720e-01	3.567e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	4.386e-27					
H2	2.193e-27	2.560e-27	-26.659	-26.592	0.067	
28.59						
Mg	4.807e-02					
Mg+2	4.497e-02	1.252e-02	-1.347	-1.902	-0.555	-
20.81						
MgSO4	3.023e-03	3.529e-03	-2.520	-2.452	0.067	
6.30						
MgHCO3+	5.531e-05	3.442e-05	-4.257	-4.463	-0.206	
6.16						
MgOH+	1.135e-05	7.936e-06	-4.945	-5.100	-0.155	
(0)						
MgCO3	8.147e-06	9.510e-06	-5.089	-5.022	0.067	-
17.10						
Na	4.450e-01					
Na+	4.428e-01	3.143e-01	-0.354	-0.503	-0.149	
0.05						
NaSO4-	2.144e-03	1.435e-03	-2.669	-2.843	-0.174	
20.88						
NaHCO3	3.003e-05	3.505e-05	-4.522	-4.455	0.067	
1.80						
NaCO3-	1.027e-05	7.603e-06	-4.989	-5.119	-0.130	
4.09						
NaOH	3.789e-17	4.423e-17	-16.421	-16.354	0.067	
(0)						
O(0)	4.265e-35					
O2	2.132e-35	2.489e-35	-34.671	-34.604	0.067	
31.40						
S(6)	1.100e-02					
SO4-2	4.747e-03	8.321e-04	-2.324	-3.080	-0.756	
19.20						
MgSO4	3.023e-03	3.529e-03	-2.520	-2.452	0.067	
6.30						
NaSO4-	2.144e-03	1.435e-03	-2.669	-2.843	-0.174	
20.88						
CaSO4	1.086e-03	1.268e-03	-2.964	-2.897	0.067	
7.96						
HSO4-	3.152e-09	2.334e-09	-8.501	-8.632	-0.130	
41.78						
CaHSO4+	2.918e-10	2.161e-10	-9.535	-9.665	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.74	-5.19	-4.45	CaSO4
Aragonite	0.13	-8.31	-8.45	CaCO3
Calcite	0.27	-8.31	-8.58	CaCO3
CO2 (g)	-3.43	-5.05	-1.63	CO2
Dolomite	1.01	-16.41	-17.42	CaMg (CO3) 2
Gypsum	-0.61	-5.21	-4.60	CaSO4:2H2O
H2 (g)	-23.46	-26.59	-3.13	H2

H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-31.62	-34.60	-2.98	O2

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
 Using pressure 1.

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

Elements	Molality	Moles
C	4.822e-04	4.822e-04
Ca	3.312e-02	3.312e-02
Cl	5.720e-01	5.720e-01
Mg	4.807e-02	4.807e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

	pH =	7.687	Charge balance
	pe =	-2.366	Adjusted to redox
equilibrium			
	Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67731
	Density (g/cm^3)	=	1.01674
	Volume (L)	=	1.01707
	Activity of water	=	0.981
	Ionic strength (mol/kgw)	=	6.721e-01
	Mass of water (kg)	=	1.000e+00
	Total alkalinity (eq/kg)	=	5.200e-04
	Total CO2 (mol/kg)	=	4.822e-04
	Temperature (°C)	=	40.00
	Pressure (atm)	=	11.00
	Electrical balance (eq)	=	1.286e-02
	Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.09
	Iterations	=	14
	Total H	=	1.110129e+02
	Total O	=	5.555167e+01

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

			Log	Log	Log
mole V	Species	Molality	Activity	Molality	Activity
cm ³ /mol					Gamma

OH-	2.338e-06	1.408e-06	-5.631	-5.851	-0.220	-
2.20						
H+	2.741e-08	2.057e-08	-7.562	-7.687	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.15						
C(-4)	5.357e-26					
CH4	5.357e-26	6.253e-26	-25.271	-25.204	0.067	
36.63						
C(4)	4.822e-04					
HCO3-	3.208e-04	2.148e-04	-3.494	-3.668	-0.174	
27.65						
MgHCO3+	5.532e-05	3.443e-05	-4.257	-4.463	-0.206	
6.19						
CaHCO3+	3.641e-05	2.499e-05	-4.439	-4.602	-0.163	
10.46						
NaHCO3	3.031e-05	3.539e-05	-4.518	-4.451	0.067	
1.80						
NaCO3-	1.028e-05	7.612e-06	-4.988	-5.119	-0.130	
4.18						
CaCO3	1.014e-05	1.183e-05	-4.994	-4.927	0.067	-
14.49						
MgCO3	8.163e-06	9.529e-06	-5.088	-5.021	0.067	-
17.02						
CO2	7.574e-06	8.842e-06	-5.121	-5.053	0.067	
35.15						
CO3-2	3.155e-06	6.340e-07	-5.501	-6.198	-0.697	-
1.58						
(CO2) 2	1.936e-12	2.261e-12	-11.713	-11.646	0.067	
70.30						
Ca	3.312e-02					
Ca+2	3.199e-02	7.708e-03	-1.495	-2.113	-0.618	-
16.39						
CaSO4	1.087e-03	1.268e-03	-2.964	-2.897	0.067	
7.99						
CaHCO3+	3.641e-05	2.499e-05	-4.439	-4.602	-0.163	
10.46						
CaCO3	1.014e-05	1.183e-05	-4.994	-4.927	0.067	-
14.49						
CaOH+	8.244e-08	6.106e-08	-7.084	-7.214	-0.130	
(0)						
CaHSO4+	2.949e-10	2.184e-10	-9.530	-9.661	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.568e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	2.371e-14					
H2	1.185e-14	1.384e-14	-13.926	-13.859	0.067	
28.59						
Mg	4.807e-02					
Mg+2	4.498e-02	1.253e-02	-1.347	-1.902	-0.555	-
20.74						
MgSO4	3.020e-03	3.526e-03	-2.520	-2.453	0.067	
6.33						
MgHCO3+	5.532e-05	3.443e-05	-4.257	-4.463	-0.206	
6.19						

MgOH+	1.127e-05	7.877e-06	-4.948	-5.104	-0.155	
(0)						
MgCO3	8.163e-06	9.529e-06	-5.088	-5.021	0.067	-
17.02						
Na	4.450e-01					
Na+	4.428e-01	3.144e-01	-0.354	-0.502	-0.149	
0.08						
NaSO4-	2.145e-03	1.436e-03	-2.669	-2.843	-0.174	
20.81						
NaHCO3	3.031e-05	3.539e-05	-4.518	-4.451	0.067	
1.80						
NaCO3-	1.028e-05	7.612e-06	-4.988	-5.119	-0.130	
4.18						
NaOH	3.789e-17	4.423e-17	-16.421	-16.354	0.067	
(0)						
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-60.146	-60.078	0.067	
31.38						
S(-2)	2.950e-22					
HS-	2.776e-22	1.672e-22	-21.557	-21.777	-0.220	
21.90						
H2S	1.735e-23	2.026e-23	-22.761	-22.693	0.067	
37.19						
S-2	1.411e-26	2.633e-27	-25.851	-26.579	-0.729	
(0)						
S(6)	1.100e-02					
SO4-2	4.748e-03	8.331e-04	-2.323	-3.079	-0.756	
19.16						
MgSO4	3.020e-03	3.526e-03	-2.520	-2.453	0.067	
6.33						
NaSO4-	2.145e-03	1.436e-03	-2.669	-2.843	-0.174	
20.81						
CaSO4	1.087e-03	1.268e-03	-2.964	-2.897	0.067	
7.99						
HSO4-	3.151e-09	2.334e-09	-8.502	-8.632	-0.130	
41.75						
CaHSO4+	2.949e-10	2.184e-10	-9.530	-9.661	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K, 11 atm)	
Anhydrite	-0.75	-5.19	-4.44	CaSO4
Aragonite	0.13	-8.31	-8.44	CaCO3
Calcite	0.26	-8.31	-8.57	CaCO3
CH4(g)	-22.29	-25.20	-2.92	CH4
CO2(g)	-3.42	-5.05	-1.63	CO2
Dolomite	0.99	-16.41	-17.40	CaMg(CO3)2
Gypsum	-0.62	-5.21	-4.59	CaSO4:2H2O
H2(g)	-10.73	-13.86	-3.13	H2
H2O(g)	-1.14	-0.01	1.14	H2O
H2S(g)	-21.50	-29.46	-7.97	H2S
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-57.09	-60.08	-2.99	O2
Sulfur	-16.59	-12.05	4.54	S

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.174 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
3\May10\phreeqc\May10_ID=14+7+5.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
3\May10\phreeqc\May10_ID=14+7+5.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.5
pe 4
redox pe
units mmol/kgw
density 1
Ca 34.68
Mg 49.78
Na 445
S(6) 11
Alkalinity 0.48 as HCO3-
Cl 572
water 1 # kg

REACTION_PRESSURE 1

14

 Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	4.800e-04	4.800e-04
Ca	3.468e-02	3.468e-02
Cl	5.720e-01	5.720e-01
Mg	4.978e-02	4.978e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	7.500
pe	=	4.000
Specific Conductance (µS/cm, 40°C)	=	67878
Density (g/cm³)	=	1.01647
Volume (L)	=	1.01744
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.784e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	4.620e-04
Total CO2 (mol/kg)	=	4.620e-04
Temperature (°C)	=	40.00
Electrical balance (eq)	=	1.944e-02
Percent error, 100*(Cat- An)/(Cat+ An)	=	1.64
Iterations	=	7
Total H	=	1.110129e+02
Total O	=	5.555160e+01

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

mole V Species cm³/mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.511e-06	9.085e-07	-5.821	-6.042	-0.221	-
2.19 H+	4.217e-08	3.162e-08	-7.375	-7.500	-0.125	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16 C(4)	4.620e-04					
HCO3-	3.096e-04	2.071e-04	-3.509	-3.684	-0.175	
27.66						

MgHCO3+	5.530e-05	3.437e-05	-4.257	-4.464	-0.207	
6.16						
CaHCO3+	3.674e-05	2.520e-05	-4.435	-4.599	-0.164	
10.44						
NaHCO3	2.889e-05	3.377e-05	-4.539	-4.471	0.068	
1.80						
CO2	1.132e-05	1.324e-05	-4.946	-4.878	0.068	
35.16						
CaCO3	6.574e-06	7.686e-06	-5.182	-5.114	0.068	-
14.56						
NaCO3-	6.381e-06	4.730e-06	-5.195	-5.325	-0.130	
4.12						
MgCO3	5.246e-06	6.133e-06	-5.280	-5.212	0.068	-
17.10						
CO3-2	1.963e-06	3.931e-07	-5.707	-6.406	-0.699	-
1.65						
(CO2) 2	4.334e-12	5.067e-12	-11.363	-11.295	0.068	
70.32						
Ca	3.468e-02					
Ca+2	3.352e-02	8.062e-03	-1.475	-2.094	-0.619	-
16.46						
CaSO4	1.118e-03	1.307e-03	-2.952	-2.884	0.068	
7.96						
CaHCO3+	3.674e-05	2.520e-05	-4.435	-4.599	-0.164	
10.44						
CaCO3	6.574e-06	7.686e-06	-5.182	-5.114	0.068	-
14.56						
CaOH+	5.601e-08	4.152e-08	-7.252	-7.382	-0.130	
(0)						
CaHSO4+	4.653e-10	3.449e-10	-9.332	-9.462	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.564e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	1.051e-26					
H2	5.253e-27	6.141e-27	-26.280	-26.212	0.068	
28.59						
Mg	4.978e-02					
Mg+2	4.663e-02	1.299e-02	-1.331	-1.887	-0.555	-
20.81						
MgSO4	3.080e-03	3.601e-03	-2.511	-2.444	0.068	
6.30						
MgHCO3+	5.530e-05	3.437e-05	-4.257	-4.464	-0.207	
6.16						
MgOH+	7.604e-06	5.312e-06	-5.119	-5.275	-0.156	
(0)						
MgCO3	5.246e-06	6.133e-06	-5.280	-5.212	0.068	-
17.10						
Na	4.450e-01					
Na+	4.429e-01	3.144e-01	-0.354	-0.502	-0.149	
0.05						
NaSO4-	2.112e-03	1.413e-03	-2.675	-2.850	-0.175	
20.92						
NaHCO3	2.889e-05	3.377e-05	-4.539	-4.471	0.068	
1.80						
NaCO3-	6.381e-06	4.730e-06	-5.195	-5.325	-0.130	
4.12						

NaOH	2.443e-17	2.856e-17	-16.612	-16.544	0.068
(0)					
O(0)	7.400e-36				
O2	3.700e-36	4.325e-36	-35.432	-35.364	0.068
31.40					
S(6)	1.100e-02				
SO4-2	4.690e-03	8.189e-04	-2.329	-3.087	-0.758
19.21					
MgSO4	3.080e-03	3.601e-03	-2.511	-2.444	0.068
6.30					
NaSO4-	2.112e-03	1.413e-03	-2.675	-2.850	-0.175
20.92					
CaSO4	1.118e-03	1.307e-03	-2.952	-2.884	0.068
7.96					
HSO4-	4.801e-09	3.558e-09	-8.319	-8.449	-0.130
41.78					
CaHSO4+	4.653e-10	3.449e-10	-9.332	-9.462	-0.130
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.73	-5.18	-4.45	CaSO4
Aragonite	-0.05	-8.50	-8.45	CaCO3
Calcite	0.08	-8.50	-8.58	CaCO3
CO2(g)	-3.25	-4.88	-1.63	CO2
Dolomite	0.63	-16.79	-17.42	CaMg(CO3)2
Gypsum	-0.60	-5.20	-4.60	CaSO4:2H2O
H2(g)	-23.08	-26.21	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-32.38	-35.36	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
C	4.620e-04	4.620e-04
Ca	3.468e-02	3.468e-02
Cl	5.720e-01	5.720e-01
Mg	4.978e-02	4.978e-02
Na	4.450e-01	4.450e-01

S 1.100e-02 1.100e-02

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

equilibrium
pH = 7.496 Charge balance
pe = -2.188 Adjusted to redox
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C) = 67879
Density (g/cm^3) = 1.01702
Volume (L) = 1.01689
Activity of water = 0.981
Ionic strength (mol/kgw) = 6.784e-01
Mass of water (kg) = 1.000e+00
Total alkalinity (eq/kg) = 4.800e-04
Total CO2 (mol/kg) = 4.620e-04
Temperature (°C) = 40.00
Pressure (atm) = 14.00
Electrical balance (eq) = 1.944e-02
Percent error, $100 * (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = 1.64
Iterations = 11
Total H = 1.110129e+02
Total O = 5.555160e+01

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

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm^3/mol						
OH-	1.510e-06	9.085e-07	-5.821	-6.042	-0.221	-
2.19						
H+	4.260e-08	3.195e-08	-7.371	-7.496	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.15						
C(-4)	1.020e-25					
CH4	1.020e-25	1.192e-25	-24.992	-24.924	0.068	
36.63						
C(4)	4.620e-04					
HCO3-	3.092e-04	2.069e-04	-3.510	-3.684	-0.175	
27.67						
MgHCO3+	5.531e-05	3.439e-05	-4.257	-4.464	-0.206	
6.20						
CaHCO3+	3.675e-05	2.521e-05	-4.435	-4.598	-0.164	
10.47						
NaHCO3	2.925e-05	3.420e-05	-4.534	-4.466	0.068	
1.80						
CO2	1.128e-05	1.319e-05	-4.948	-4.880	0.068	
35.15						
CaCO3	6.594e-06	7.708e-06	-5.181	-5.113	0.068	-
14.47						
NaCO3-	6.386e-06	4.734e-06	-5.195	-5.325	-0.130	
4.24						

MgCO3	5.257e-06	6.145e-06	-5.279	-5.211	0.068	-
17.00						
CO3-2	1.968e-06	3.945e-07	-5.706	-6.404	-0.698	-
1.54						
(CO2)2	4.302e-12	5.030e-12	-11.366	-11.298	0.068	
70.30						
Ca	3.468e-02					
Ca+2	3.352e-02	8.071e-03	-1.475	-2.093	-0.618	-
16.37						
CaSO4	1.118e-03	1.307e-03	-2.952	-2.884	0.068	
8.00						
CaHCO3+	3.675e-05	2.521e-05	-4.435	-4.598	-0.164	
10.47						
CaCO3	6.594e-06	7.708e-06	-5.181	-5.113	0.068	-
14.47						
CaOH+	5.554e-08	4.118e-08	-7.255	-7.385	-0.130	
(0)						
CaHSO4+	4.720e-10	3.499e-10	-9.326	-9.456	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.565e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	2.511e-14					
H2	1.256e-14	1.468e-14	-13.901	-13.833	0.068	
28.59						
Mg	4.978e-02					
Mg+2	4.664e-02	1.300e-02	-1.331	-1.886	-0.555	-
20.71						
MgSO4	3.076e-03	3.597e-03	-2.512	-2.444	0.068	
6.34						
MgHCO3+	5.531e-05	3.439e-05	-4.257	-4.464	-0.206	
6.20						
MgOH+	7.523e-06	5.257e-06	-5.124	-5.279	-0.156	
(0)						
MgCO3	5.257e-06	6.145e-06	-5.279	-5.211	0.068	-
17.00						
Na	4.450e-01					
Na+	4.429e-01	3.145e-01	-0.354	-0.502	-0.149	
0.09						
NaSO4-	2.114e-03	1.414e-03	-2.675	-2.849	-0.175	
20.83						
NaHCO3	2.925e-05	3.420e-05	-4.534	-4.466	0.068	
1.80						
NaCO3-	6.386e-06	4.734e-06	-5.195	-5.325	-0.130	
4.24						
NaOH	2.442e-17	2.854e-17	-16.612	-16.544	0.068	
(0)						
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-60.200	-60.132	0.068	
31.37						
S(-2)	5.932e-22					
HS-	5.409e-22	3.253e-22	-21.267	-21.488	-0.221	
21.90						
H2S	5.228e-23	6.112e-23	-22.282	-22.214	0.068	
37.19						
S-2	1.778e-26	3.308e-27	-25.750	-26.480	-0.730	
(0)						

S(6)	1.100e-02					
SO4-2	4.692e-03	8.202e-04	-2.329	-3.086	-0.757	
19.16						
MgSO4	3.076e-03	3.597e-03	-2.512	-2.444	0.068	
6.34						
NaSO4-	2.114e-03	1.414e-03	-2.675	-2.849	-0.175	
20.83						
CaSO4	1.118e-03	1.307e-03	-2.952	-2.884	0.068	
8.00						
HSO4-	4.802e-09	3.560e-09	-8.319	-8.449	-0.130	
41.75						
CaHSO4+	4.720e-10	3.499e-10	-9.326	-9.456	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K, 14 atm)	
Anhydrite	-0.74	-5.18	-4.44	CaSO4
Aragonite	-0.06	-8.50	-8.43	CaCO3
Calcite	0.07	-8.50	-8.57	CaCO3
CH4(g)	-22.00	-24.92	-2.92	CH4
CO2(g)	-3.25	-4.88	-1.63	CO2
Dolomite	0.61	-16.79	-17.40	CaMg(CO3)2
Gypsum	-0.61	-5.20	-4.59	CaSO4:2H2O
H2(g)	-10.70	-13.83	-3.13	H2
H2O(g)	-1.14	-0.01	1.13	H2O
H2S(g)	-21.02	-28.98	-7.97	H2S
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-57.14	-60.13	-2.99	O2
Sulfur	-16.14	-11.60	4.54	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.163 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
3\May10_CC\phreeqc\May10_ID=14+7+5+5.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
3\May10_CC\phreeqc\May10_ID=14+7+5+5.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.55
pe 4
redox pe
units mmol/kgw
density 1
Ca 36.10
Mg 51.31
Na 445
S(6) 11
Alkalinity 0.36 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
37

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	3.600e-04	3.600e-04
Ca	3.610e-02	3.610e-02
Cl	5.720e-01	5.720e-01
Mg	5.131e-02	5.131e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH = 7.550
pe = 4.000

Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C) = 68011
 Density (g/cm^3) = 1.01661
 Volume (L) = 1.01738
 Activity of water = 0.981
 Ionic strength (mol/kgw) = $6.840\text{e-}01$
 Mass of water (kg) = $1.000\text{e+}00$
 Total carbon (mol/kg) = $3.400\text{e-}04$
 Total CO_2 (mol/kg) = $3.400\text{e-}04$
 Temperature ($^\circ\text{C}$) = 40.00
 Electrical balance (eq) = $2.546\text{e-}02$
 Percent error, $100 * (\text{Cat-}|\text{An}|) / (\text{Cat+}|\text{An}|)$ = 2.13
 Iterations = 6
 Total H = $1.110128\text{e+}02$
 Total O = $5.555124\text{e+}01$

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

--

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm^3/mol						
OH-	$1.697\text{e-}06$	$1.019\text{e-}06$	-5.770	-5.992	-0.221	-
2.18						
H+	$3.760\text{e-}08$	$2.818\text{e-}08$	-7.425	-7.550	-0.125	
0.00						
H ₂ O	$5.551\text{e+}01$	$9.811\text{e-}01$	1.744	-0.008	0.000	
18.16						
C(4)	$3.400\text{e-}04$					
HCO ₃ -	$2.254\text{e-}04$	$1.507\text{e-}04$	-3.647	-3.822	-0.175	
27.68						
MgHCO ₃ +	$4.157\text{e-}05$	$2.581\text{e-}05$	-4.381	-4.588	-0.207	
6.16						
CaHCO ₃ +	$2.785\text{e-}05$	$1.909\text{e-}05$	-4.555	-4.719	-0.164	
10.44						
NaHCO ₃	$2.100\text{e-}05$	$2.458\text{e-}05$	-4.678	-4.609	0.068	
1.80						
CO ₂	$7.335\text{e-}06$	$8.586\text{e-}06$	-5.135	-5.066	0.068	
35.16						
CaCO ₃	$5.580\text{e-}06$	$6.532\text{e-}06$	-5.253	-5.185	0.068	-
14.56						
NaCO ₃ -	$5.207\text{e-}06$	$3.862\text{e-}06$	-5.283	-5.413	-0.130	
4.15						
MgCO ₃	$4.414\text{e-}06$	$5.167\text{e-}06$	-5.355	-5.287	0.068	-
17.10						
CO ₃ -2	$1.607\text{e-}06$	$3.209\text{e-}07$	-5.794	-6.494	-0.700	-
1.64						
(CO ₂) ₂	$1.821\text{e-}12$	$2.131\text{e-}12$	-11.740	-11.671	0.068	
70.32						
Ca	$3.610\text{e-}02$					
Ca+2	$3.492\text{e-}02$	$8.393\text{e-}03$	-1.457	-2.076	-0.619	-
16.45						
CaSO ₄	$1.146\text{e-}03$	$1.341\text{e-}03$	-2.941	-2.872	0.068	
7.96						
CaHCO ₃ +	$2.785\text{e-}05$	$1.909\text{e-}05$	-4.555	-4.719	-0.164	
10.44						

CaCO3	5.580e-06	6.532e-06	-5.253	-5.185	0.068	-
14.56						
CaOH+	6.536e-08	4.849e-08	-7.185	-7.314	-0.130	
(0)						
CaHSO4+	4.253e-10	3.155e-10	-9.371	-9.501	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.561e-01	-0.243	-0.448	-0.206	
19.08						
H(0)	8.334e-27					
H2	4.167e-27	4.878e-27	-26.380	-26.312	0.068	
28.59						
Mg	5.131e-02					
Mg+2	4.813e-02	1.340e-02	-1.318	-1.873	-0.555	-
20.80						
MgSO4	3.130e-03	3.664e-03	-2.504	-2.436	0.068	
6.30						
MgHCO3+	4.157e-05	2.581e-05	-4.381	-4.588	-0.207	
6.16						
MgOH+	8.809e-06	6.151e-06	-5.055	-5.211	-0.156	
(0)						
MgCO3	4.414e-06	5.167e-06	-5.355	-5.287	0.068	-
17.10						
Na	4.450e-01					
Na+	4.429e-01	3.145e-01	-0.354	-0.502	-0.149	
0.05						
NaSO4-	2.084e-03	1.393e-03	-2.681	-2.856	-0.175	
20.95						
NaHCO3	2.100e-05	2.458e-05	-4.678	-4.609	0.068	
1.80						
NaCO3-	5.207e-06	3.862e-06	-5.283	-5.413	-0.130	
4.15						
NaOH	2.738e-17	3.206e-17	-16.562	-16.494	0.068	
(0)						
O(0)	1.171e-35					
O2	5.856e-36	6.854e-36	-35.232	-35.164	0.068	
31.40						
S(6)	1.100e-02					
SO4-2	4.640e-03	8.074e-04	-2.334	-3.093	-0.759	
19.23						
MgSO4	3.130e-03	3.664e-03	-2.504	-2.436	0.068	
6.30						
NaSO4-	2.084e-03	1.393e-03	-2.681	-2.856	-0.175	
20.95						
CaSO4	1.146e-03	1.341e-03	-2.941	-2.872	0.068	
7.96						
HSO4-	4.215e-09	3.127e-09	-8.375	-8.505	-0.130	
41.79						
CaHSO4+	4.253e-10	3.155e-10	-9.371	-9.501	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K, 1 atm)
Anhydrite	-0.72	-5.17	-4.45 CaSO4

Aragonite	-0.12	-8.57	-8.45	CaCO3
Calcite	0.01	-8.57	-8.58	CaCO3
CO2(g)	-3.44	-5.07	-1.63	CO2
Dolomite	0.49	-16.94	-17.42	CaMg(CO3)2
Gypsum	-0.59	-5.19	-4.60	CaSO4:2H2O
H2(g)	-23.18	-26.31	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-32.18	-35.16	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
 Using pressure 1.

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

--

Elements	Molality	Moles
C	3.400e-04	3.400e-04
Ca	3.610e-02	3.610e-02
Cl	5.720e-01	5.720e-01
Mg	5.131e-02	5.131e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	7.539	Charge balance
	pe =	-2.330	Adjusted to redox
equilibrium			
	Specific Conductance (µS/cm, 40°C)	=	68013
	Density (g/cm³)	=	1.01813
	Volume (L)	=	1.01586
	Activity of water	=	0.981
	Ionic strength (mol/kgw)	=	6.840e-01
	Mass of water (kg)	=	1.000e+00
	Total alkalinity (eq/kg)	=	3.600e-04
	Total CO2 (mol/kg)	=	3.400e-04
	Temperature (°C)	=	40.00
	Pressure (atm)	=	37.00
	Electrical balance (eq)	=	2.546e-02
Percent error, 100*(Cat- An)/(Cat+ An)		=	2.13
	Iterations	=	15
	Total H	=	1.110128e+02
	Total O	=	5.555124e+01

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

--

mole V Species cm ³ /mol	Molality	Activity	Log		Log		Gamma
			Molality	Activity	Molality	Activity	
OH-	1.700e-06	1.022e-06	-5.770	-5.990	-0.221	-	
2.17							
H+	3.855e-08	2.892e-08	-7.414	-7.539	-0.125		
0.00							
H2O	5.551e+01	9.811e-01	1.744	-0.008	0.000		
18.13							
C(-4)	3.911e-25						
CH4	3.911e-25	4.578e-25	-24.408	-24.339	0.068		
36.66							
C(4)	3.400e-04						
HCO3-	2.246e-04	1.503e-04	-3.649	-3.823	-0.175		
27.71							
MgHCO3+	4.159e-05	2.585e-05	-4.381	-4.588	-0.207		
6.27							
CaHCO3+	2.787e-05	1.912e-05	-4.555	-4.719	-0.164		
10.52							
NaHCO3	2.173e-05	2.544e-05	-4.663	-4.594	0.068		
1.80							
CO2	7.239e-06	8.474e-06	-5.140	-5.072	0.068		
35.13							
CaCO3	5.640e-06	6.602e-06	-5.249	-5.180	0.068	-	
14.31							
NaCO3-	5.230e-06	3.882e-06	-5.281	-5.411	-0.129		
4.47							
MgCO3	4.450e-06	5.210e-06	-5.352	-5.283	0.068	-	
16.83							
CO3-2	1.622e-06	3.249e-07	-5.790	-6.488	-0.698	-	
1.35							
(CO2) 2	1.774e-12	2.076e-12	-11.751	-11.683	0.068		
70.26							
Ca	3.610e-02						
Ca+2	3.492e-02	8.419e-03	-1.457	-2.075	-0.618	-	
16.21							
CaSO4	1.146e-03	1.341e-03	-2.941	-2.872	0.068		
8.06							
CaHCO3+	2.787e-05	1.912e-05	-4.555	-4.719	-0.164		
10.52							
CaCO3	5.640e-06	6.602e-06	-5.249	-5.180	0.068	-	
14.31							
CaOH+	6.404e-08	4.753e-08	-7.194	-7.323	-0.129		
(0)							
CaHSO4+	4.411e-10	3.274e-10	-9.355	-9.485	-0.129		
(0)							
Cl	5.720e-01						
Cl-	5.720e-01	3.564e-01	-0.243	-0.448	-0.205		
19.09							
H(0)	3.855e-14						
H2	1.928e-14	2.256e-14	-13.715	-13.647	0.068		
28.58							

Mg	5.131e-02					
Mg+2	4.814e-02	1.344e-02	-1.318	-1.872	-0.554	-
20.53						
MgSO4	3.119e-03	3.651e-03	-2.506	-2.438	0.068	
6.40						
MgHCO3+	4.159e-05	2.585e-05	-4.381	-4.588	-0.207	
6.27						
MgOH+	8.578e-06	5.994e-06	-5.067	-5.222	-0.156	
(0)						
MgCO3	4.450e-06	5.210e-06	-5.352	-5.283	0.068	-
16.83						
Na	4.450e-01					
Na+	4.429e-01	3.148e-01	-0.354	-0.502	-0.148	
0.16						
NaSO4-	2.089e-03	1.398e-03	-2.680	-2.855	-0.175	
20.71						
NaHCO3	2.173e-05	2.544e-05	-4.663	-4.594	0.068	
1.80						
NaCO3-	5.230e-06	3.882e-06	-5.281	-5.411	-0.129	
4.47						
NaOH	2.741e-17	3.208e-17	-16.562	-16.494	0.068	
(0)						
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-60.595	-60.526	0.068	
31.33						
S(-2)	3.041e-21					
HS-	2.799e-21	1.683e-21	-20.553	-20.774	-0.221	
21.90						
H2S	2.412e-22	2.823e-22	-21.618	-21.549	0.068	
37.15						
S-2	1.037e-25	1.928e-26	-24.984	-25.715	-0.731	
(0)						
S(6)	1.100e-02					
SO4-2	4.646e-03	8.109e-04	-2.333	-3.091	-0.758	
19.08						
MgSO4	3.119e-03	3.651e-03	-2.506	-2.438	0.068	
6.40						
NaSO4-	2.089e-03	1.398e-03	-2.680	-2.855	-0.175	
20.71						
CaSO4	1.146e-03	1.341e-03	-2.941	-2.872	0.068	
8.06						
HSO4-	4.205e-09	3.121e-09	-8.376	-8.506	-0.129	
41.68						
CaHSO4+	4.411e-10	3.274e-10	-9.355	-9.485	-0.129	
(0)						

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

Phase	SI**	log IAP	log K(313 K, 37 atm)	
Anhydrite	-0.74	-5.17	-4.43	CaSO4
Aragonite	-0.15	-8.56	-8.41	CaCO3
Calcite	-0.02	-8.56	-8.55	CaCO3
CH4 (g)	-21.41	-24.34	-2.93	CH4
CO2 (g)	-3.43	-5.07	-1.65	CO2
Dolomite	0.44	-16.92	-17.36	CaMg (CO3) 2

Gypsum	-0.61	-5.18	-4.58	CaSO4:2H2O
H2 (g)	-10.50	-13.65	-3.15	H2
H2O (g)	-1.14	-0.01	1.13	H2O
H2S (g)	-20.34	-28.31	-7.98	H2S
Halite	-2.54	-0.95	1.59	NaCl
O2 (g)	-57.52	-60.53	-3.00	O2
Sulfur	-15.66	-11.13	4.53	S

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.161 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
3\May10_CC\phreeqc\May10_ID=14+7+5+5+5.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
3\May10_CC\phreeqc\May10_ID=14+7+5+5+5.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.9
pe 4
redox pe
units mmol/kgw
density 1

```

Ca      33.82
Mg      49.45
Na      445
S(6)    11
Alkalinity 0.4 as HCO3-
Cl      572
water   1 # kg
REACTION_PRESSURE 1
61

```

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	4.000e-04	4.000e-04
Ca	3.382e-02	3.382e-02
Cl	5.720e-01	5.720e-01
Mg	4.945e-02	4.945e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

```

pH = 7.900
pe = 4.000
Specific Conductance (µS/cm, 40°C) = 67819
Density (g/cm³) = 1.01641
Volume (L) = 1.01745
Activity of water = 0.981
Ionic strength (mol/kgw) = 6.760e-01
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 3.446e-04
Total CO2 (mol/kg) = 3.446e-04
Temperature (°C) = 40.00
Electrical balance (eq) = 1.714e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.45
Iterations = 6
Total H = 1.110128e+02
Total O = 5.555127e+01

```

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

mole V Species cm ³ /mol	Molality	Activity	Log	Log	Log	-
			Molality	Activity	Gamma	
OH- 2.19	3.794e-06	2.282e-06	-5.421	-5.642	-0.221	-

H+	1.679e-08	1.259e-08	-7.775	-7.900	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(4)	3.446e-04					
HCO3-	2.205e-04	1.475e-04	-3.657	-3.831	-0.175	
27.66						
MgHCO3+	3.910e-05	2.431e-05	-4.408	-4.614	-0.206	
6.16						
CaHCO3+	2.552e-05	1.751e-05	-4.593	-4.757	-0.164	
10.44						
NaHCO3	2.059e-05	2.405e-05	-4.686	-4.619	0.068	
1.80						
CaCO3	1.148e-05	1.341e-05	-4.940	-4.872	0.068	-
14.56						
NaCO3-	1.142e-05	8.461e-06	-4.942	-5.073	-0.130	
4.11						
MgCO3	9.325e-06	1.090e-05	-5.030	-4.963	0.068	-
17.10						
CO3-2	3.509e-06	7.033e-07	-5.455	-6.153	-0.698	-
1.66						
CO2	3.212e-06	3.754e-06	-5.493	-5.426	0.068	
35.16						
(CO2)2	3.486e-13	4.074e-13	-12.458	-12.390	0.068	
70.32						
Ca	3.382e-02					
Ca+2	3.269e-02	7.865e-03	-1.486	-2.104	-0.619	-
16.46						
CaSO4	1.096e-03	1.281e-03	-2.960	-2.892	0.068	
7.96						
CaHCO3+	2.552e-05	1.751e-05	-4.593	-4.757	-0.164	
10.44						
CaCO3	1.148e-05	1.341e-05	-4.940	-4.872	0.068	-
14.56						
CaOH+	1.373e-07	1.017e-07	-6.862	-6.993	-0.130	
(0)						
CaHSO4+	1.817e-10	1.346e-10	-9.741	-9.871	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.565e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	1.666e-27					
H2	8.330e-28	9.733e-28	-27.079	-27.012	0.068	
28.59						
Mg	4.945e-02					
Mg+2	4.631e-02	1.290e-02	-1.334	-1.890	-0.555	-
20.81						
MgSO4	3.076e-03	3.594e-03	-2.512	-2.444	0.068	
6.30						
MgHCO3+	3.910e-05	2.431e-05	-4.408	-4.614	-0.206	
6.16						
MgOH+	1.896e-05	1.325e-05	-4.722	-4.878	-0.156	
(0)						
MgCO3	9.325e-06	1.090e-05	-5.030	-4.963	0.068	-
17.10						
Na	4.450e-01					

Na+	4.428e-01	3.144e-01	-0.354	-0.503	-0.149
0.05					
NaSO4-	2.122e-03	1.420e-03	-2.673	-2.848	-0.175
20.90					
NaHCO3	2.059e-05	2.405e-05	-4.686	-4.619	0.068
1.80					
NaCO3-	1.142e-05	8.461e-06	-4.942	-5.073	-0.130
4.11					
NaOH	6.140e-17	7.175e-17	-16.212	-16.144	0.068
(0)					
O(0)	2.948e-34				
O2	1.474e-34	1.722e-34	-33.832	-33.764	0.068
31.40					
S(6)	1.100e-02				
SO4-2	4.706e-03	8.230e-04	-2.327	-3.085	-0.757
19.21					
MgSO4	3.076e-03	3.594e-03	-2.512	-2.444	0.068
6.30					
NaSO4-	2.122e-03	1.420e-03	-2.673	-2.848	-0.175
20.90					
CaSO4	1.096e-03	1.281e-03	-2.960	-2.892	0.068
7.96					
HSO4-	1.921e-09	1.424e-09	-8.716	-8.847	-0.130
41.78					
CaHSO4+	1.817e-10	1.346e-10	-9.741	-9.871	-0.130
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.74	-5.19	-4.45	CaSO4
Aragonite	0.19	-8.26	-8.45	CaCO3
Calcite	0.32	-8.26	-8.58	CaCO3
CO2(g)	-3.80	-5.43	-1.63	CO2
Dolomite	1.12	-16.30	-17.42	CaMg(CO3)2
Gypsum	-0.61	-5.21	-4.60	CaSO4:2H2O
H2(g)	-23.88	-27.01	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-30.78	-33.76	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
C	3.446e-04	3.446e-04
Ca	3.382e-02	3.382e-02
Cl	5.720e-01	5.720e-01
Mg	4.945e-02	4.945e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	7.884	Charge balance
	pe =	-2.526	Adjusted to redox
equilibrium			
	Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67820
	Density (g/cm^3)	=	1.01894
	Volume (L)	=	1.01493
	Activity of water	=	0.981
	Ionic strength (mol/kgw)	=	6.761e-01
	Mass of water (kg)	=	1.000e+00
	Total alkalinity (eq/kg)	=	4.000e-04
	Total CO2 (mol/kg)	=	3.446e-04
	Temperature (°C)	=	40.00
	Pressure (atm)	=	61.00
	Electrical balance (eq)	=	1.714e-02
	Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.45
	Iterations	=	13
	Total H	=	1.110128e+02
	Total O	=	5.555127e+01

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	Gamma
			Molality	Activity		
OH-	3.825e-06	2.305e-06	-5.417	-5.637	-0.220	-
2.18						
H+	1.741e-08	1.307e-08	-7.759	-7.884	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.11						
C(-4)	1.044e-26					
CH4	1.044e-26	1.220e-26	-25.981	-25.914	0.068	
36.68						
C(4)	3.446e-04					
HCO3-	2.188e-04	1.466e-04	-3.660	-3.834	-0.174	
27.71						
MgHCO3+	3.909e-05	2.434e-05	-4.408	-4.614	-0.206	
6.34						
CaHCO3+	2.552e-05	1.753e-05	-4.593	-4.756	-0.163	
10.56						

NaHCO3	2.177e-05	2.544e-05	-4.662	-4.595	0.068	
1.80						
CaCO3	1.173e-05	1.370e-05	-4.931	-4.863	0.068	-
14.15						
NaCO3-	1.154e-05	8.562e-06	-4.938	-5.067	-0.130	
4.63						
MgCO3	9.487e-06	1.109e-05	-5.023	-4.955	0.068	-
16.66						
CO3-2	3.575e-06	7.199e-07	-5.447	-6.143	-0.696	-
1.17						
CO2	3.122e-06	3.648e-06	-5.506	-5.438	0.068	
35.11						
(CO2) 2	3.293e-13	3.848e-13	-12.482	-12.415	0.068	
70.22						
Ca	3.382e-02					
Ca+2	3.269e-02	7.905e-03	-1.486	-2.102	-0.616	-
16.06						
CaSO4	1.096e-03	1.281e-03	-2.960	-2.892	0.068	
8.12						
CaHCO3+	2.552e-05	1.753e-05	-4.593	-4.756	-0.163	
10.56						
CaCO3	1.173e-05	1.370e-05	-4.931	-4.863	0.068	-
14.15						
CaOH+	1.334e-07	9.896e-08	-6.875	-7.005	-0.130	
(0)						
CaHSO4+	1.920e-10	1.424e-10	-9.717	-9.846	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.571e-01	-0.243	-0.447	-0.205	
19.09						
H(0)	1.893e-14					
H2	9.463e-15	1.106e-14	-14.024	-13.956	0.068	
28.56						
Mg	4.945e-02					
Mg+2	4.633e-02	1.296e-02	-1.334	-1.887	-0.553	-
20.36						
MgSO4	3.057e-03	3.572e-03	-2.515	-2.447	0.068	
6.46						
MgHCO3+	3.909e-05	2.434e-05	-4.408	-4.614	-0.206	
6.34						
MgOH+	1.824e-05	1.276e-05	-4.739	-4.894	-0.155	
(0)						
MgCO3	9.487e-06	1.109e-05	-5.023	-4.955	0.068	-
16.66						
Na	4.450e-01					
Na+	4.428e-01	3.148e-01	-0.354	-0.502	-0.148	
0.23						
NaSO4-	2.131e-03	1.427e-03	-2.671	-2.845	-0.174	
20.51						
NaHCO3	2.177e-05	2.544e-05	-4.662	-4.595	0.068	
1.80						
NaCO3-	1.154e-05	8.562e-06	-4.938	-5.067	-0.130	
4.63						
NaOH	6.182e-17	7.223e-17	-16.209	-16.141	0.068	
(0)						
O(0)	0.000e+00					

O2	0.000e+00	0.000e+00	-59.995	-59.928	0.068
31.28					
S(-2)	8.011e-23				
HS-	7.713e-23	4.647e-23	-22.113	-22.333	-0.220
21.90					
H2S	2.973e-24	3.474e-24	-23.527	-23.459	0.068
37.10					
S-2	6.426e-27	1.202e-27	-26.192	-26.920	-0.728
(0)					
S(6)	1.100e-02				
SO4-2	4.716e-03	8.288e-04	-2.326	-3.082	-0.755
18.96					
MgSO4	3.057e-03	3.572e-03	-2.515	-2.447	0.068
6.46					
NaSO4-	2.131e-03	1.427e-03	-2.671	-2.845	-0.174
20.51					
CaSO4	1.096e-03	1.281e-03	-2.960	-2.892	0.068
8.12					
HSO4-	1.904e-09	1.412e-09	-8.720	-8.850	-0.130
41.61					
CaHSO4+	1.920e-10	1.424e-10	-9.717	-9.846	-0.130
(0)					

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

Phase	SI**	log IAP	log K(313 K, 61 atm)	
Anhydrite	-0.78	-5.18	-4.41	CaSO4
Aragonite	0.15	-8.24	-8.39	CaCO3
Calcite	0.28	-8.24	-8.52	CaCO3
CH4(g)	-22.96	-25.91	-2.95	CH4
CO2(g)	-3.78	-5.44	-1.66	CO2
Dolomite	1.04	-16.27	-17.32	CaMg(CO3)2
Gypsum	-0.64	-5.20	-4.56	CaSO4:2H2O
H2(g)	-10.80	-13.96	-3.16	H2
H2O(g)	-1.13	-0.01	1.12	H2O
H2S(g)	-22.23	-30.22	-7.98	H2S
Halite	-2.54	-0.95	1.59	NaCl
O2(g)	-56.91	-59.93	-3.02	O2
Sulfur	-17.25	-12.74	4.51	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.151 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
3\April17_SP\phreeqc\Apr17_ID=0.5_Measure.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
3\April17_SP\phreeqc\Apr17_ID=0.5_Measure.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 30
Mg 42
Na 445
S(6) 11
Alkalinity 1 as HCO3-
Cl 572
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	1.000e-03	1.000e-03
Ca	3.000e-02	3.000e-02
Cl	5.720e-01	5.720e-01
Mg	4.200e-02	4.200e-02
Na	4.450e-01	4.450e-01

S(6)

1.100e-02 1.100e-02

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

pH = 8.200
 pe = 4.000
 Specific Conductance (µS/cm, 40°C) = 67333
 Density (g/cm³) = 1.01589
 Volume (L) = 1.01766
 Activity of water = 0.981
 Ionic strength (mol/kgw) = 6.546e-01
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 8.160e-04
 Total CO2 (mol/kg) = 8.160e-04
 Temperature (°C) = 40.00
 Electrical balance (eq) = -6.000e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.52
 Iterations = 6
 Total H = 1.110131e+02
 Total O = 5.555270e+01

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

mole V Species cm³/mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	7.539e-06	4.554e-06	-5.123	-5.342	-0.219	-
2.23 H+	8.402e-09	6.310e-09	-8.076	-8.200	-0.124	
0.00 H2O	5.551e+01	9.814e-01	1.744	-0.008	0.000	
18.16 C(4)	8.160e-04					
HCO3-	4.935e-04	3.311e-04	-3.307	-3.480	-0.173	
27.60 MgHCO3+	7.382e-05	4.607e-05	-4.132	-4.337	-0.205	
6.16 NaCO3-	5.124e-05	3.786e-05	-4.290	-4.422	-0.131	
3.99 CaHCO3+	5.064e-05	3.482e-05	-4.296	-4.458	-0.163	
10.44 NaHCO3	4.639e-05	5.394e-05	-4.334	-4.268	0.065	
1.80 CaCO3	4.578e-05	5.322e-05	-4.339	-4.274	0.065	-
14.56 MgCO3	3.543e-05	4.120e-05	-4.451	-4.385	0.065	-
17.10 CO3-2	1.555e-05	3.149e-06	-4.808	-5.502	-0.693	-
1.71 CO2	3.631e-06	4.221e-06	-5.440	-5.375	0.065	
35.16 (CO2)2	4.432e-13	5.153e-13	-12.353	-12.288	0.065	
70.32						

Ca	3.000e-02						
Ca+2	2.887e-02	6.969e-03	-1.540	-2.157	-0.617	-	
16.48							
CaSO4	1.038e-03	1.207e-03	-2.984	-2.918	0.065		
7.96							
CaHCO3+	5.064e-05	3.482e-05	-4.296	-4.458	-0.163		
10.44							
CaCO3	4.578e-05	5.322e-05	-4.339	-4.274	0.065	-	
14.56							
CaOH+	2.435e-07	1.799e-07	-6.614	-6.745	-0.131		
(0)							
CaHSO4+	8.605e-11	6.357e-11	-10.065	-10.197	-0.131		
(0)							
Cl	5.720e-01						
Cl-	5.720e-01	3.577e-01	-0.243	-0.447	-0.204		
19.07							
H(0)	4.205e-28						
H2	2.103e-28	2.445e-28	-27.677	-27.612	0.065		
28.59							
Mg	4.200e-02						
Mg+2	3.908e-02	1.089e-02	-1.408	-1.963	-0.555	-	
20.83							
MgSO4	2.776e-03	3.227e-03	-2.557	-2.491	0.065		
6.30							
MgHCO3+	7.382e-05	4.607e-05	-4.132	-4.337	-0.205		
6.16							
MgCO3	3.543e-05	4.120e-05	-4.451	-4.385	0.065	-	
17.10							
MgOH+	3.189e-05	2.233e-05	-4.496	-4.651	-0.155		
(0)							
Na	4.450e-01						
Na+	4.427e-01	3.141e-01	-0.354	-0.503	-0.149		
0.04							
NaSO4-	2.248e-03	1.508e-03	-2.648	-2.821	-0.173		
20.77							
NaCO3-	5.124e-05	3.786e-05	-4.290	-4.422	-0.131		
3.99							
NaHCO3	4.639e-05	5.394e-05	-4.334	-4.268	0.065		
1.80							
NaOH	1.230e-16	1.431e-16	-15.910	-15.844	0.065		
(0)							
O(0)	4.696e-33						
O2	2.348e-33	2.730e-33	-32.629	-32.564	0.065		
31.40							
S(6)	1.100e-02						
SO4-2	4.938e-03	8.752e-04	-2.306	-3.058	-0.751		
19.15							
MgSO4	2.776e-03	3.227e-03	-2.557	-2.491	0.065		
6.30							
NaSO4-	2.248e-03	1.508e-03	-2.648	-2.821	-0.173		
20.77							
CaSO4	1.038e-03	1.207e-03	-2.984	-2.918	0.065		
7.96							
HSO4-	1.027e-09	7.588e-10	-8.988	-9.120	-0.131		
41.77							
CaHSO4+	8.605e-11	6.357e-11	-10.065	-10.197	-0.131		
(0)							

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

--

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.76	-5.21	-4.45	CaSO4
Aragonite	0.79	-7.66	-8.45	CaCO3
Calcite	0.92	-7.66	-8.58	CaCO3
CO2(g)	-3.75	-5.37	-1.63	CO2
Dolomite	2.30	-15.12	-17.42	CaMg(CO3)2
Gypsum	-0.63	-5.23	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-29.58	-32.56	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.145 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
3\April17_SP\phreeqc\Apr17_ID=0_theory.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
3\April17_SP\phreeqc\Apr17_ID=0_theory.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67832
Density (g/cm^3)	=	1.01647
Volume (L)	=	1.01750
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.753e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.989e-03
Total CO2 (mol/kg)	=	1.989e-03
Temperature (°C)	=	40.00
Electrical balance (eq)	=	1.460e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23
Iterations	=	7
Total H	=	1.110141e+02
Total O	=	5.555622e+01

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

mole V Species cm ³ /mol	Molality	Activity	Log		Log	
			Molality	Activity	Gamma	
OH-	7.568e-06	4.553e-06	-5.121	-5.342	-0.221	-
2.19						
H+	8.413e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(4)	1.989e-03					
HCO3-	1.160e-03	7.764e-04	-2.935	-3.110	-0.174	
27.66						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
CO3-2	3.684e-05	7.386e-06	-4.434	-5.132	-0.698	-
1.66						
CO2	8.476e-06	9.902e-06	-5.072	-5.004	0.068	
35.16						
(CO2)2	2.427e-12	2.835e-12	-11.615	-11.547	0.068	
70.32						
Ca	3.500e-02					
Ca+2	3.360e-02	8.086e-03	-1.474	-2.092	-0.619	-
16.46						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
CaOH+	2.817e-07	2.087e-07	-6.550	-6.681	-0.130	
(0)						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	4.185e-28					
H2	2.093e-28	2.445e-28	-27.679	-27.612	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.244e-02	-1.350	-1.905	-0.555	-
20.81						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						

MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
MgOH+	3.650e-05	2.551e-05	-4.438	-4.593	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.142e-01	-0.354	-0.503	-0.149	
0.05						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
NaOH	1.225e-16	1.431e-16	-15.912	-15.844	0.068	
(0)						
O(0)	4.672e-33					
O2	2.336e-33	2.729e-33	-32.632	-32.564	0.068	
31.40						
S(6)	1.100e-02					
SO4-2	4.738e-03	8.290e-04	-2.324	-3.081	-0.757	
19.21						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
HSO4-	9.700e-10	7.187e-10	-9.013	-9.143	-0.130	
41.78						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.72	-5.17	-4.45	CaSO4
Aragonite	1.22	-7.22	-8.45	CaCO3
Calcite	1.36	-7.22	-8.58	CaCO3
CO2(g)	-3.38	-5.00	-1.63	CO2
Dolomite	3.16	-14.26	-17.42	CaMg(CO3)2
Gypsum	-0.59	-5.19	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-29.58	-32.56	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

Reading input data for simulation 2.

End of Run after 0.133 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
3\April17_SP\phreeqc\Apr17_ID=14_Measure.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
3\April17_SP\phreeqc\Apr17_ID=14_Measure.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.49
pe 4
redox pe
units mmol/kgw
density 1
Ca 34.13
Mg 48
Na 445
S(6) 11
Alkalinity 0.92 as HCO3-
Cl 572
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	9.200e-04	9.200e-04
Ca	3.413e-02	3.413e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

--

	pH	=	7.490
	pe	=	4.000
Specific Conductance	($\mu\text{S}/\text{cm}$, 40°C)	=	67785
	Density (g/cm^3)	=	1.01638
	Volume (L)	=	1.01749
	Activity of water	=	0.981
	Ionic strength (mol/kgw)	=	6.740e-01
	Mass of water (kg)	=	1.000e+00
	Total carbon (mol/kg)	=	8.961e-04
	Total CO2 (mol/kg)	=	8.961e-04
	Temperature (°C)	=	40.00
	Electrical balance (eq)	=	1.434e-02
Percent error,	$100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.21
	Iterations	=	8
	Total H	=	1.110133e+02
	Total O	=	5.555289e+01

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	1.475e-06	8.878e-07	-5.831	-6.052	-0.221	-
2.20						
H+	4.314e-08	3.236e-08	-7.365	-7.490	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(4)	8.961e-04					
HCO3-	6.046e-04	4.046e-04	-3.219	-3.393	-0.174	
27.65						
MgHCO3+	1.039e-04	6.463e-05	-3.983	-4.190	-0.206	
6.16						
CaHCO3+	7.054e-05	4.840e-05	-4.152	-4.315	-0.164	
10.44						
NaHCO3	5.649e-05	6.597e-05	-4.248	-4.181	0.067	
1.80						
CO2	2.266e-05	2.647e-05	-4.645	-4.577	0.067	
35.16						
CaCO3	1.235e-05	1.443e-05	-4.908	-4.841	0.067	-
14.56						

NaCO3-	1.219e-05	9.028e-06	-4.914	-5.044	-0.130	
4.10						
MgCO3	9.648e-06	1.127e-05	-5.016	-4.948	0.067	-
17.10						
CO3-2	3.741e-06	7.505e-07	-5.427	-6.125	-0.698	-
1.66						
(CO2)2	1.734e-11	2.025e-11	-10.761	-10.694	0.067	
70.32						
Ca	3.413e-02					
Ca+2	3.293e-02	7.926e-03	-1.482	-2.101	-0.619	-
16.46						
CaSO4	1.115e-03	1.302e-03	-2.953	-2.885	0.067	
7.96						
CaHCO3+	7.054e-05	4.840e-05	-4.152	-4.315	-0.164	
10.44						
CaCO3	1.235e-05	1.443e-05	-4.908	-4.841	0.067	-
14.56						
CaOH+	5.385e-08	3.989e-08	-7.269	-7.399	-0.130	
(0)						
CaHSO4+	4.747e-10	3.516e-10	-9.324	-9.454	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	1.101e-26					
H2	5.506e-27	6.430e-27	-26.259	-26.192	0.067	
28.59						
Mg	4.800e-02					
Mg+2	4.487e-02	1.250e-02	-1.348	-1.903	-0.555	-
20.81						
MgSO4	3.007e-03	3.512e-03	-2.522	-2.454	0.067	
6.30						
MgHCO3+	1.039e-04	6.463e-05	-3.983	-4.190	-0.206	
6.16						
MgCO3	9.648e-06	1.127e-05	-5.016	-4.948	0.067	-
17.10						
MgOH+	7.148e-06	4.996e-06	-5.146	-5.301	-0.156	
(0)						
Na	4.450e-01					
Na+	4.428e-01	3.143e-01	-0.354	-0.503	-0.149	
0.05						
NaSO4-	2.139e-03	1.431e-03	-2.670	-2.844	-0.174	
20.89						
NaHCO3	5.649e-05	6.597e-05	-4.248	-4.181	0.067	
1.80						
NaCO3-	1.219e-05	9.028e-06	-4.914	-5.044	-0.130	
4.10						
NaOH	2.390e-17	2.791e-17	-16.622	-16.554	0.067	
(0)						
O(0)	6.756e-36					
O2	3.378e-36	3.945e-36	-35.471	-35.404	0.067	
31.40						
S(6)	1.100e-02					
SO4-2	4.739e-03	8.299e-04	-2.324	-3.081	-0.757	
19.20						
MgSO4	3.007e-03	3.512e-03	-2.522	-2.454	0.067	
6.30						

NaSO4-	2.139e-03	1.431e-03	-2.670	-2.844	-0.174
20.89					
CaSO4	1.115e-03	1.302e-03	-2.953	-2.885	0.067
7.96					
HSO4-	4.981e-09	3.690e-09	-8.303	-8.433	-0.130
41.78					
CaHSO4+	4.747e-10	3.516e-10	-9.324	-9.454	-0.130
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.73	-5.18	-4.45	CaSO4
Aragonite	0.22	-8.23	-8.45	CaCO3
Calcite	0.35	-8.23	-8.58	CaCO3
CO2(g)	-2.95	-4.58	-1.63	CO2
Dolomite	1.17	-16.25	-17.42	CaMg(CO3)2
Gypsum	-0.60	-5.20	-4.60	CaSO4:2H2O
H2(g)	-23.06	-26.19	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-32.42	-35.40	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.139 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
3\April17_SP\phreeqc\Apr17_ID=14+7_Measure.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
3\April17_SP\phreeqc\Apr17_ID=14+7_Measure.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.54
pe 4
redox pe
units mmol/kgw
density 1
Ca 30.82
Mg 43.77
Na 445
S(6) 11
Alkalinity 0.96 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
11

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	9.600e-04	9.600e-04
Ca	3.082e-02	3.082e-02
Cl	5.720e-01	5.720e-01
Mg	4.377e-02	4.377e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	7.540
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67448
Density (g/cm^3)	=	1.01602
Volume (L)	=	1.01762
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.596e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	9.298e-04
Total CO2 (mol/kg)	=	9.298e-04

Temperature (°C) = 40.00
 Electrical balance (eq) = -7.800e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.07
 Iterations = 7
 Total H = 1.110133e+02
 Total O = 5.555299e+01

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

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.651e-06	9.963e-07	-5.782	-6.002	-0.219	-
2.22						
H+	3.841e-08	2.884e-08	-7.416	-7.540	-0.124	
0.00						
H2O	5.551e+01	9.813e-01	1.744	-0.008	0.000	
18.16						
C(4)	9.298e-04					
HCO3-	6.387e-04	4.282e-04	-3.195	-3.368	-0.174	
27.61						
MgHCO3+	9.975e-05	6.220e-05	-4.001	-4.206	-0.205	
6.16						
CaHCO3+	6.735e-05	4.628e-05	-4.172	-4.335	-0.163	
10.44						
NaHCO3	5.995e-05	6.978e-05	-4.222	-4.156	0.066	
1.80						
CO2	2.144e-05	2.496e-05	-4.669	-4.603	0.066	
35.16						
NaCO3-	1.449e-05	1.071e-05	-4.839	-4.970	-0.131	
4.02						
CaCO3	1.330e-05	1.548e-05	-4.876	-4.810	0.066	-
14.56						
MgCO3	1.045e-05	1.217e-05	-4.981	-4.915	0.066	-
17.10						
CO3-2	4.411e-06	8.912e-07	-5.355	-6.050	-0.695	-
1.69						
(CO2)2	1.547e-11	1.801e-11	-10.810	-10.744	0.066	
70.32						
Ca	3.082e-02					
Ca+2	2.969e-02	7.162e-03	-1.527	-2.145	-0.618	-
16.47						
CaSO4	1.050e-03	1.222e-03	-2.979	-2.913	0.066	
7.96						
CaHCO3+	6.735e-05	4.628e-05	-4.172	-4.335	-0.163	
10.44						
CaCO3	1.330e-05	1.548e-05	-4.876	-4.810	0.066	-
14.56						
CaOH+	5.470e-08	4.044e-08	-7.262	-7.393	-0.131	
(0)						
CaHSO4+	3.980e-10	2.943e-10	-9.400	-9.531	-0.131	
(0)						
Cl	5.720e-01					

Cl-	5.720e-01	3.574e-01	-0.243	-0.447	-0.204	
19.07						
H(0)	8.776e-27					
H2	4.388e-27	5.108e-27	-26.358	-26.292	0.066	
28.59						
Mg	4.377e-02					
Mg+2	4.080e-02	1.137e-02	-1.389	-1.944	-0.555	-
20.82						
MgSO4	2.851e-03	3.319e-03	-2.545	-2.479	0.066	
6.30						
MgHCO3+	9.975e-05	6.220e-05	-4.001	-4.206	-0.205	
6.16						
MgCO3	1.045e-05	1.217e-05	-4.981	-4.915	0.066	-
17.10						
MgOH+	7.285e-06	5.099e-06	-5.138	-5.293	-0.155	
(0)						
Na	4.450e-01					
Na+	4.427e-01	3.142e-01	-0.354	-0.503	-0.149	
0.04						
NaSO4-	2.217e-03	1.487e-03	-2.654	-2.828	-0.174	
20.80						
NaHCO3	5.995e-05	6.978e-05	-4.222	-4.156	0.066	
1.80						
NaCO3-	1.449e-05	1.071e-05	-4.839	-4.970	-0.131	
4.02						
NaOH	2.689e-17	3.130e-17	-16.570	-16.504	0.066	
(0)						
O(0)	1.075e-35					
O2	5.373e-36	6.254e-36	-35.270	-35.204	0.066	
31.40						
S(6)	1.100e-02					
SO4-2	4.881e-03	8.624e-04	-2.311	-3.064	-0.753	
19.16						
MgSO4	2.851e-03	3.319e-03	-2.545	-2.479	0.066	
6.30						
NaSO4-	2.217e-03	1.487e-03	-2.654	-2.828	-0.174	
20.80						
CaSO4	1.050e-03	1.222e-03	-2.979	-2.913	0.066	
7.96						
HSO4-	4.623e-09	3.417e-09	-8.335	-8.466	-0.131	
41.77						
CaHSO4+	3.980e-10	2.943e-10	-9.400	-9.531	-0.131	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.76	-5.21	-4.45	CaSO4
Aragonite	0.25	-8.20	-8.45	CaCO3
Calcite	0.38	-8.20	-8.58	CaCO3
CO2(g)	-2.98	-4.60	-1.63	CO2
Dolomite	1.23	-16.19	-17.42	CaMg(CO3)2
Gypsum	-0.63	-5.23	-4.60	CaSO4:2H2O
H2(g)	-23.16	-26.29	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O

Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-32.22	-35.20	-2.98	O2

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
 Using pressure 1.

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

Elements	Molality	Moles
C	9.298e-04	9.298e-04
Ca	3.082e-02	3.082e-02
Cl	5.720e-01	5.720e-01
Mg	4.377e-02	4.377e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

	pH =	7.536	Charge balance
	pe =	9.184	Adjusted to redox
equilibrium			
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67448	
Density (g/cm^3)	=	1.01644	
Volume (L)	=	1.01720	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.596e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	9.600e-04	
Total CO2 (mol/kg)	=	9.298e-04	
Temperature (°C)	=	40.00	
Pressure (atm)	=	11.00	
Electrical balance (eq)	=	-7.800e-04	
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	-0.07	
Iterations	=	11	
Total H	=	1.110133e+02	
Total O	=	5.555299e+01	

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

			Log	Log	Log	
mole V	Species	Molality	Activity	Molality	Activity	Gamma
cm^3/mol						

OH-	1.649e-06	9.955e-07	-5.783	-6.002	-0.219	-
2.22						
H+	3.875e-08	2.909e-08	-7.412	-7.536	-0.124	
0.00						
H2O	5.551e+01	9.813e-01	1.744	-0.008	0.000	
18.15						
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-116.015	-115.949	0.066	
36.63						
C(4)	9.298e-04					
HCO3-	6.381e-04	4.279e-04	-3.195	-3.369	-0.174	
27.62						
MgHCO3+	9.977e-05	6.223e-05	-4.001	-4.206	-0.205	
6.19						
CaHCO3+	6.736e-05	4.630e-05	-4.172	-4.334	-0.163	
10.46						
NaHCO3	6.052e-05	7.045e-05	-4.218	-4.152	0.066	
1.80						
CO2	2.140e-05	2.491e-05	-4.670	-4.604	0.066	
35.15						
NaCO3-	1.449e-05	1.071e-05	-4.839	-4.970	-0.131	
4.10						
CaCO3	1.331e-05	1.550e-05	-4.876	-4.810	0.066	-
14.49						
MgCO3	1.046e-05	1.218e-05	-4.980	-4.914	0.066	-
17.02						
CO3-2	4.416e-06	8.928e-07	-5.355	-6.049	-0.694	-
1.61						
(CO2) 2	1.541e-11	1.794e-11	-10.812	-10.746	0.066	
70.30						
Ca	3.082e-02					
Ca+2	2.969e-02	7.168e-03	-1.527	-2.145	-0.617	-
16.40						
CaSO4	1.050e-03	1.222e-03	-2.979	-2.913	0.066	
7.99						
CaHCO3+	6.736e-05	4.630e-05	-4.172	-4.334	-0.163	
10.46						
CaCO3	1.331e-05	1.550e-05	-4.876	-4.810	0.066	-
14.49						
CaOH+	5.430e-08	4.015e-08	-7.265	-7.396	-0.131	
(0)						
CaHSO4+	4.027e-10	2.978e-10	-9.395	-9.526	-0.131	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.575e-01	-0.243	-0.447	-0.204	
19.07						
H(0)	3.780e-37					
H2	1.890e-37	2.200e-37	-36.723	-36.658	0.066	
28.59						
Mg	4.377e-02					
Mg+2	4.080e-02	1.137e-02	-1.389	-1.944	-0.555	-
20.75						
MgSO4	2.848e-03	3.316e-03	-2.545	-2.479	0.066	
6.33						
MgHCO3+	9.977e-05	6.223e-05	-4.001	-4.206	-0.205	
6.19						

MgCO3	1.046e-05	1.218e-05	-4.980	-4.914	0.066	-
17.02						
MgOH+	7.219e-06	5.054e-06	-5.142	-5.296	-0.155	
(0)						
Na	4.450e-01					
Na+	4.427e-01	3.143e-01	-0.354	-0.503	-0.149	
0.07						
NaSO4-	2.219e-03	1.488e-03	-2.654	-2.827	-0.174	
20.73						
NaHCO3	6.052e-05	7.045e-05	-4.218	-4.152	0.066	
1.80						
NaCO3-	1.449e-05	1.071e-05	-4.839	-4.970	-0.131	
4.10						
NaOH	2.685e-17	3.126e-17	-16.571	-16.505	0.066	
(0)						
O(0)	5.674e-15					
O2	2.837e-15	3.303e-15	-14.547	-14.481	0.066	
31.38						
S(-2)	0.000e+00					
HS-	0.000e+00	0.000e+00	-112.586	-112.805	-0.219	
21.89						
H2S	0.000e+00	0.000e+00	-113.637	-113.571	0.066	
37.19						
S-2	0.000e+00	0.000e+00	-117.032	-117.759	-0.726	
(0)						
S(6)	1.100e-02					
SO4-2	4.883e-03	8.634e-04	-2.311	-3.064	-0.752	
19.12						
MgSO4	2.848e-03	3.316e-03	-2.545	-2.479	0.066	
6.33						
NaSO4-	2.219e-03	1.488e-03	-2.654	-2.827	-0.174	
20.73						
CaSO4	1.050e-03	1.222e-03	-2.979	-2.913	0.066	
7.99						
HSO4-	4.627e-09	3.421e-09	-8.335	-8.466	-0.131	
41.74						
CaHSO4+	4.027e-10	2.978e-10	-9.395	-9.526	-0.131	
(0)						

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

Phase	SI**	log IAP	log K(313 K, 11 atm)	
Anhydrite	-0.76	-5.21	-4.44	CaSO4
Aragonite	0.24	-8.19	-8.44	CaCO3
Calcite	0.38	-8.19	-8.57	CaCO3
CH4(g)	-113.03	-115.95	-2.92	CH4
CO2(g)	-2.97	-4.60	-1.63	CO2
Dolomite	1.22	-16.19	-17.40	CaMg(CO3)2
Gypsum	-0.63	-5.22	-4.59	CaSO4:2H2O
H2(g)	-33.53	-36.66	-3.13	H2
H2O(g)	-1.14	-0.01	1.14	H2O
H2S(g)	-112.38	-120.34	-7.97	H2S
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-11.49	-14.48	-2.99	O2
Sulfur	-84.67	-80.13	4.54	S

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.156 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
3\April17_SP\phreeqc\Apr17_ID=14+7+5_Measure.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
3\April17_SP\phreeqc\Apr17_ID=14+7+5_Measure.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.5
pe 4
redox pe
units mmol/kgw
density 1
Ca 36.31
Mg 50.42
Na 445
S(6) 11
Alkalinity 0.64 as HCO3-
Cl 572
water 1 # kg

REACTION_PRESSURE 1

14

 Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	6.400e-04	6.400e-04
Ca	3.631e-02	3.631e-02
Cl	5.720e-01	5.720e-01
Mg	5.042e-02	5.042e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

	pH	=	7.500
	pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)		=	67991
Density (g/cm^3)		=	1.01659
Volume (L)		=	1.01740
Activity of water		=	0.981
Ionic strength (mol/kgw)		=	6.827e-01
Mass of water (kg)		=	1.000e+00
Total carbon (mol/kg)		=	6.185e-04
Total CO2 (mol/kg)		=	6.185e-04
Temperature (°C)		=	40.00
Electrical balance (eq)		=	2.382e-02
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$		=	2.00
	Iterations	=	7
	Total H	=	1.110130e+02
	Total O	=	5.555207e+01

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

mole V Species cm^3/mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.512e-06	9.085e-07	-5.820	-6.042	-0.221	-
2.18 H+	4.218e-08	3.162e-08	-7.375	-7.500	-0.125	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16 C(4)	6.185e-04					
HCO3-	4.120e-04	2.755e-04	-3.385	-3.560	-0.175	
27.68						

MgHCO3+	7.457e-05	4.632e-05	-4.127	-4.334	-0.207	
6.16						
CaHCO3+	5.116e-05	3.507e-05	-4.291	-4.455	-0.164	
10.44						
NaHCO3	3.839e-05	4.493e-05	-4.416	-4.347	0.068	
1.80						
CO2	1.505e-05	1.761e-05	-4.823	-4.754	0.068	
35.16						
CaCO3	9.140e-06	1.070e-05	-5.039	-4.971	0.068	-
14.56						
NaCO3-	8.483e-06	6.292e-06	-5.071	-5.201	-0.130	
4.15						
MgCO3	7.062e-06	8.264e-06	-5.151	-5.083	0.068	-
17.10						
CO3-2	2.617e-06	5.229e-07	-5.582	-6.282	-0.699	-
1.64						
(CO2) 2	7.662e-12	8.966e-12	-11.116	-11.047	0.068	
70.32						
Ca	3.631e-02					
Ca+2	3.509e-02	8.435e-03	-1.455	-2.074	-0.619	-
16.45						
CaSO4	1.158e-03	1.355e-03	-2.936	-2.868	0.068	
7.96						
CaHCO3+	5.116e-05	3.507e-05	-4.291	-4.455	-0.164	
10.44						
CaCO3	9.140e-06	1.070e-05	-5.039	-4.971	0.068	-
14.56						
CaOH+	5.856e-08	4.344e-08	-7.232	-7.362	-0.130	
(0)						
CaHSO4+	4.821e-10	3.576e-10	-9.317	-9.447	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.562e-01	-0.243	-0.448	-0.206	
19.08						
H(0)	1.050e-26					
H2	5.248e-27	6.141e-27	-26.280	-26.212	0.068	
28.59						
Mg	5.042e-02					
Mg+2	4.724e-02	1.315e-02	-1.326	-1.881	-0.555	-
20.80						
MgSO4	3.089e-03	3.615e-03	-2.510	-2.442	0.068	
6.30						
MgHCO3+	7.457e-05	4.632e-05	-4.127	-4.334	-0.207	
6.16						
MgOH+	7.706e-06	5.381e-06	-5.113	-5.269	-0.156	
(0)						
MgCO3	7.062e-06	8.264e-06	-5.151	-5.083	0.068	-
17.10						
Na	4.450e-01					
Na+	4.429e-01	3.145e-01	-0.354	-0.502	-0.149	
0.05						
NaSO4-	2.094e-03	1.400e-03	-2.679	-2.854	-0.175	
20.95						
NaHCO3	3.839e-05	4.493e-05	-4.416	-4.347	0.068	
1.80						
NaCO3-	8.483e-06	6.292e-06	-5.071	-5.201	-0.130	
4.15						

NaOH	2.441e-17	2.857e-17	-16.612	-16.544	0.068
(0)					
O(0)	7.391e-36				
O2	3.696e-36	4.325e-36	-35.432	-35.364	0.068
31.40					
S(6)	1.100e-02				
SO4-2	4.659e-03	8.114e-04	-2.332	-3.091	-0.759
19.23					
MgSO4	3.089e-03	3.615e-03	-2.510	-2.442	0.068
6.30					
NaSO4-	2.094e-03	1.400e-03	-2.679	-2.854	-0.175
20.95					
CaSO4	1.158e-03	1.355e-03	-2.936	-2.868	0.068
7.96					
HSO4-	4.754e-09	3.526e-09	-8.323	-8.453	-0.130
41.79					
CaHSO4+	4.821e-10	3.576e-10	-9.317	-9.447	-0.130
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.71	-5.16	-4.45	CaSO4
Aragonite	0.09	-8.36	-8.45	CaCO3
Calcite	0.22	-8.36	-8.58	CaCO3
CO2(g)	-3.13	-4.75	-1.63	CO2
Dolomite	0.90	-16.52	-17.42	CaMg(CO3)2
Gypsum	-0.58	-5.18	-4.60	CaSO4:2H2O
H2(g)	-23.08	-26.21	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-32.38	-35.36	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
 Using pressure 1.

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

Elements	Molality	Moles
C	6.185e-04	6.185e-04
Ca	3.631e-02	3.631e-02
Cl	5.720e-01	5.720e-01
Mg	5.042e-02	5.042e-02
Na	4.450e-01	4.450e-01

S 1.100e-02 1.100e-02

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

equilibrium

	pH	=	7.495	Charge balance
	pe	=	-2.156	Adjusted to redox
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67991		
Density (g/cm^3)	=	1.01714		
Volume (L)	=	1.01685		
Activity of water	=	0.981		
Ionic strength (mol/kgw)	=	6.828e-01		
Mass of water (kg)	=	1.000e+00		
Total alkalinity (eq/kg)	=	6.400e-04		
Total CO2 (mol/kg)	=	6.185e-04		
Temperature (°C)	=	40.00		
Pressure (atm)	=	14.00		
Electrical balance (eq)	=	2.382e-02		
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	2.00		
Iterations	=	13		
Total H	=	1.110130e+02		
Total O	=	5.555207e+01		

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

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm^3/mol						
OH-	1.511e-06	9.080e-07	-5.821	-6.042	-0.221	-
2.18						
H+	4.263e-08	3.197e-08	-7.370	-7.495	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.15						
C(-4)	7.596e-26					
CH4	7.596e-26	8.889e-26	-25.119	-25.051	0.068	
36.63						
C(4)	6.185e-04					
HCO3-	4.115e-04	2.752e-04	-3.386	-3.560	-0.175	
27.69						
MgHCO3+	7.459e-05	4.634e-05	-4.127	-4.334	-0.207	
6.20						
CaHCO3+	5.117e-05	3.509e-05	-4.291	-4.455	-0.164	
10.47						
NaHCO3	3.888e-05	4.549e-05	-4.410	-4.342	0.068	
1.80						
CO2	1.500e-05	1.755e-05	-4.824	-4.756	0.068	
35.15						
CaCO3	9.162e-06	1.072e-05	-5.038	-4.970	0.068	-
14.47						
NaCO3-	8.485e-06	6.295e-06	-5.071	-5.201	-0.130	
4.26						

MgCO3	7.072e-06	8.276e-06	-5.150	-5.082	0.068	-
17.00						
CO3-2	2.622e-06	5.245e-07	-5.581	-6.280	-0.699	-
1.53						
(CO2)2	7.613e-12	8.909e-12	-11.118	-11.050	0.068	
70.30						
Ca	3.631e-02					
Ca+2	3.509e-02	8.445e-03	-1.455	-2.073	-0.619	-
16.36						
CaSO4	1.158e-03	1.355e-03	-2.936	-2.868	0.068	
8.00						
CaHCO3+	5.117e-05	3.509e-05	-4.291	-4.455	-0.164	
10.47						
CaCO3	9.162e-06	1.072e-05	-5.038	-4.970	0.068	-
14.47						
CaOH+	5.804e-08	4.306e-08	-7.236	-7.366	-0.130	
(0)						
CaHSO4+	4.892e-10	3.629e-10	-9.310	-9.440	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.563e-01	-0.243	-0.448	-0.206	
19.09						
H(0)	2.171e-14					
H2	1.085e-14	1.270e-14	-13.964	-13.896	0.068	
28.59						
Mg	5.042e-02					
Mg+2	4.725e-02	1.317e-02	-1.326	-1.880	-0.555	-
20.70						
MgSO4	3.085e-03	3.610e-03	-2.511	-2.442	0.068	
6.34						
MgHCO3+	7.459e-05	4.634e-05	-4.127	-4.334	-0.207	
6.20						
MgOH+	7.620e-06	5.323e-06	-5.118	-5.274	-0.156	
(0)						
MgCO3	7.072e-06	8.276e-06	-5.150	-5.082	0.068	-
17.00						
Na	4.450e-01					
Na+	4.429e-01	3.146e-01	-0.354	-0.502	-0.149	
0.09						
NaSO4-	2.096e-03	1.402e-03	-2.679	-2.853	-0.175	
20.86						
NaHCO3	3.888e-05	4.549e-05	-4.410	-4.342	0.068	
1.80						
NaCO3-	8.485e-06	6.295e-06	-5.071	-5.201	-0.130	
4.26						
NaOH	2.438e-17	2.853e-17	-16.613	-16.545	0.068	
(0)						
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-60.075	-60.007	0.068	
31.37						
S(-2)	3.298e-22					
HS-	3.007e-22	1.807e-22	-21.522	-21.743	-0.221	
21.91						
H2S	2.903e-23	3.397e-23	-22.537	-22.469	0.068	
37.19						
S-2	9.892e-27	1.837e-27	-26.005	-26.736	-0.731	
(0)						

S(6)	1.100e-02					
SO4-2	4.661e-03	8.127e-04	-2.331	-3.090	-0.759	
19.17						
MgSO4	3.085e-03	3.610e-03	-2.511	-2.442	0.068	
6.34						
NaSO4-	2.096e-03	1.402e-03	-2.679	-2.853	-0.175	
20.86						
CaSO4	1.158e-03	1.355e-03	-2.936	-2.868	0.068	
8.00						
HSO4-	4.757e-09	3.529e-09	-8.323	-8.452	-0.130	
41.75						
CaHSO4+	4.892e-10	3.629e-10	-9.310	-9.440	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K, 14 atm)	
Anhydrite	-0.72	-5.16	-4.44	CaSO4
Aragonite	0.08	-8.35	-8.43	CaCO3
Calcite	0.21	-8.35	-8.57	CaCO3
CH4(g)	-22.13	-25.05	-2.92	CH4
CO2(g)	-3.12	-4.76	-1.63	CO2
Dolomite	0.88	-16.51	-17.40	CaMg(CO3)2
Gypsum	-0.59	-5.18	-4.59	CaSO4:2H2O
H2(g)	-10.76	-13.90	-3.13	H2
H2O(g)	-1.14	-0.01	1.13	H2O
H2S(g)	-21.27	-29.24	-7.97	H2S
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-57.02	-60.01	-2.99	O2
Sulfur	-16.33	-11.79	4.54	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

 Reading input data for simulation 2.

 End of Run after 0.164 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
 3\April17_SP\phreeqc\Apr17_ID=14+7+5+5_Measure.pqi
 Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\4) Results\Story
 3\April17_SP\phreeqc\Apr17_ID=14+7+5+5_Measure.pqo
 Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
 15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.72
pe 4
redox pe
units mmol/kgw
density 1
Ca 34.11
Mg 48.38
Na 445
S(6) 11
Alkalinity 0.48 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
37

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	4.800e-04	4.800e-04
Ca	3.411e-02	3.411e-02
Cl	5.720e-01	5.720e-01
Mg	4.838e-02	4.838e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH = 7.720
pe = 4.000

Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C) = 67794
 Density (g/cm^3) = 1.01638
 Volume (L) = 1.01747
 Activity of water = 0.981
 Ionic strength (mol/kgw) = $6.746\text{e-}01$
 Mass of water (kg) = $1.000\text{e+}00$
 Total carbon (mol/kg) = $4.405\text{e-}04$
 Total CO_2 (mol/kg) = $4.405\text{e-}04$
 Temperature ($^\circ\text{C}$) = 40.00
 Electrical balance (eq) = $1.550\text{e-}02$
 Percent error, $100 * (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = 1.31
 Iterations = 6
 Total H = $1.110129\text{e+}02$
 Total O = $5.555155\text{e+}01$

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

--

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm^3/mol						
OH-	$2.506\text{e-}06$	$1.508\text{e-}06$	-5.601	-5.822	-0.221	-
2.19						
H+	$2.540\text{e-}08$	$1.905\text{e-}08$	-7.595	-7.720	-0.125	
0.00						
H ₂ O	$5.551\text{e+}01$	$9.812\text{e-}01$	1.744	-0.008	0.000	
18.16						
C(4)	$4.405\text{e-}04$					
HCO ₃ -	$2.913\text{e-}04$	$1.949\text{e-}04$	-3.536	-3.710	-0.174	
27.65						
MgHCO ₃ +	$5.051\text{e-}05$	$3.142\text{e-}05$	-4.297	-4.503	-0.206	
6.16						
CaHCO ₃ +	$3.400\text{e-}05$	$2.333\text{e-}05$	-4.469	-4.632	-0.164	
10.44						
NaHCO ₃	$2.721\text{e-}05$	$3.178\text{e-}05$	-4.565	-4.498	0.067	
1.80						
CaCO ₃	$1.011\text{e-}05$	$1.181\text{e-}05$	-4.995	-4.928	0.067	-
14.56						
NaCO ₃ -	$9.970\text{e-}06$	$7.386\text{e-}06$	-5.001	-5.132	-0.130	
4.10						
MgCO ₃	$7.964\text{e-}06$	$9.302\text{e-}06$	-5.099	-5.031	0.067	-
17.10						
CO ₂	$6.427\text{e-}06$	$7.507\text{e-}06$	-5.192	-5.125	0.067	
35.16						
CO ₃ -2	$3.061\text{e-}06$	$6.140\text{e-}07$	-5.514	-6.212	-0.698	-
1.66						
(CO ₂) ₂	$1.395\text{e-}12$	$1.629\text{e-}12$	-11.855	-11.788	0.067	
70.32						
Ca	$3.411\text{e-}02$					
Ca+2	$3.295\text{e-}02$	$7.931\text{e-}03$	-1.482	-2.101	-0.619	-
16.46						
CaSO ₄	$1.112\text{e-}03$	$1.299\text{e-}03$	-2.954	-2.886	0.067	
7.96						
CaHCO ₃ +	$3.400\text{e-}05$	$2.333\text{e-}05$	-4.469	-4.632	-0.164	
10.44						

CaCO3	1.011e-05	1.181e-05	-4.995	-4.928	0.067	-
14.56						
CaOH+	9.149e-08	6.778e-08	-7.039	-7.169	-0.130	
(0)						
CaHSO4+	2.789e-10	2.066e-10	-9.555	-9.685	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	3.818e-27					
H2	1.909e-27	2.230e-27	-26.719	-26.652	0.067	
28.59						
Mg	4.838e-02					
Mg+2	4.528e-02	1.261e-02	-1.344	-1.899	-0.555	-
20.81						
MgSO4	3.026e-03	3.534e-03	-2.519	-2.452	0.067	
6.30						
MgHCO3+	5.051e-05	3.142e-05	-4.297	-4.503	-0.206	
6.16						
MgOH+	1.225e-05	8.562e-06	-4.912	-5.067	-0.156	
(0)						
MgCO3	7.964e-06	9.302e-06	-5.099	-5.031	0.067	-
17.10						
Na	4.450e-01					
Na+	4.428e-01	3.144e-01	-0.354	-0.503	-0.149	
0.05						
NaSO4-	2.133e-03	1.428e-03	-2.671	-2.845	-0.174	
20.90						
NaHCO3	2.721e-05	3.178e-05	-4.565	-4.498	0.067	
1.80						
NaCO3-	9.970e-06	7.386e-06	-5.001	-5.132	-0.130	
4.10						
NaOH	4.058e-17	4.740e-17	-16.392	-16.324	0.067	
(0)						
O(0)	5.618e-35					
O2	2.809e-35	3.281e-35	-34.551	-34.484	0.067	
31.40						
S(6)	1.100e-02					
SO4-2	4.729e-03	8.276e-04	-2.325	-3.082	-0.757	
19.21						
MgSO4	3.026e-03	3.534e-03	-2.519	-2.452	0.067	
6.30						
NaSO4-	2.133e-03	1.428e-03	-2.671	-2.845	-0.174	
20.90						
CaSO4	1.112e-03	1.299e-03	-2.954	-2.886	0.067	
7.96						
HSO4-	2.925e-09	2.167e-09	-8.534	-8.664	-0.130	
41.78						
CaHSO4+	2.789e-10	2.066e-10	-9.555	-9.685	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K, 1 atm)
Anhydrite	-0.73	-5.18	-4.45 CaSO4

Aragonite	0.13	-8.31	-8.45	CaCO3
Calcite	0.27	-8.31	-8.58	CaCO3
CO2(g)	-3.50	-5.12	-1.63	CO2
Dolomite	1.00	-16.42	-17.42	CaMg(CO3)2
Gypsum	-0.60	-5.20	-4.60	CaSO4:2H2O
H2(g)	-23.52	-26.65	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-31.50	-34.48	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
 Using pressure 1.

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

--

Elements	Molality	Moles
C	4.405e-04	4.405e-04
Ca	3.411e-02	3.411e-02
Cl	5.720e-01	5.720e-01
Mg	4.838e-02	4.838e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	7.709	Charge balance
	pe =	-2.194	Adjusted to redox
equilibrium			
	Specific Conductance (µS/cm, 40°C)	=	67796
	Density (g/cm³)	=	1.01790
	Volume (L)	=	1.01595
	Activity of water	=	0.981
	Ionic strength (mol/kgw)	=	6.747e-01
	Mass of water (kg)	=	1.000e+00
	Total alkalinity (eq/kg)	=	4.800e-04
	Total CO2 (mol/kg)	=	4.405e-04
	Temperature (°C)	=	40.00
	Pressure (atm)	=	37.00
	Electrical balance (eq)	=	1.550e-02
Percent error, 100*(Cat- An)/(Cat+ An)		=	1.31
	Iterations	=	11
	Total H	=	1.110129e+02
	Total O	=	5.555155e+01

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

--

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	2.510e-06	1.512e-06	-5.600	-5.820	-0.220	-
2.19						
H+	2.605e-08	1.955e-08	-7.584	-7.709	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.13						
C(-4)	1.221e-27					
CH4	1.221e-27	1.426e-27	-26.913	-26.846	0.067	
36.66						
C(4)	4.405e-04					
HCO3-	2.901e-04	1.943e-04	-3.537	-3.712	-0.174	
27.68						
MgHCO3+	5.053e-05	3.145e-05	-4.296	-4.502	-0.206	
6.27						
CaHCO3+	3.402e-05	2.336e-05	-4.468	-4.632	-0.163	
10.51						
NaHCO3	2.815e-05	3.289e-05	-4.550	-4.483	0.067	
1.80						
CaCO3	1.021e-05	1.193e-05	-4.991	-4.923	0.067	-
14.31						
NaCO3-	1.001e-05	7.421e-06	-4.999	-5.130	-0.130	
4.42						
MgCO3	8.026e-06	9.375e-06	-5.095	-5.028	0.067	-
16.83						
CO2	6.342e-06	7.408e-06	-5.198	-5.130	0.067	
35.13						
CO3-2	3.088e-06	6.212e-07	-5.510	-6.207	-0.696	-
1.37						
(CO2) 2	1.358e-12	1.587e-12	-11.867	-11.799	0.067	
70.26						
Ca	3.411e-02					
Ca+2	3.295e-02	7.955e-03	-1.482	-2.099	-0.617	-
16.22						
CaSO4	1.112e-03	1.299e-03	-2.954	-2.886	0.067	
8.06						
CaHCO3+	3.402e-05	2.336e-05	-4.468	-4.632	-0.163	
10.51						
CaCO3	1.021e-05	1.193e-05	-4.991	-4.923	0.067	-
14.31						
CaOH+	8.962e-08	6.643e-08	-7.048	-7.178	-0.130	
(0)						
CaHSO4+	2.893e-10	2.144e-10	-9.539	-9.669	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.569e-01	-0.243	-0.447	-0.205	
19.08						
H(0)	9.439e-15					
H2	4.719e-15	5.513e-15	-14.326	-14.259	0.067	
28.58						

Mg	4.838e-02						
Mg+2	4.529e-02	1.265e-02	-1.344	-1.898	-0.554	-	
20.54							
MgSO4	3.015e-03	3.522e-03	-2.521	-2.453	0.067		
6.40							
MgHCO3+	5.053e-05	3.145e-05	-4.296	-4.502	-0.206		
6.27							
MgOH+	1.193e-05	8.342e-06	-4.923	-5.079	-0.155		
(0)							
MgCO3	8.026e-06	9.375e-06	-5.095	-5.028	0.067	-	
16.83							
Na	4.450e-01						
Na+	4.428e-01	3.146e-01	-0.354	-0.502	-0.148		
0.16							
NaSO4-	2.138e-03	1.432e-03	-2.670	-2.844	-0.174		
20.65							
NaHCO3	2.815e-05	3.289e-05	-4.550	-4.483	0.067		
1.80							
NaCO3-	1.001e-05	7.421e-06	-4.999	-5.130	-0.130		
4.42							
NaOH	4.061e-17	4.743e-17	-16.391	-16.324	0.067		
(0)							
O(0)	0.000e+00						
O2	0.000e+00	0.000e+00	-59.369	-59.302	0.067		
31.33							
S(-2)	7.300e-24						
HS-	6.897e-24	4.154e-24	-23.161	-23.382	-0.220		
21.90							
H2S	4.033e-25	4.711e-25	-24.394	-24.327	0.067		
37.15							
S-2	3.767e-28	7.037e-29	-27.424	-28.153	-0.729		
(0)							
S(6)	1.100e-02						
SO4-2	4.734e-03	8.312e-04	-2.325	-3.080	-0.756		
19.05							
MgSO4	3.015e-03	3.522e-03	-2.521	-2.453	0.067		
6.40							
NaSO4-	2.138e-03	1.432e-03	-2.670	-2.844	-0.174		
20.65							
CaSO4	1.112e-03	1.299e-03	-2.954	-2.886	0.067		
8.06							
HSO4-	2.918e-09	2.163e-09	-8.535	-8.665	-0.130		
41.68							
CaHSO4+	2.893e-10	2.144e-10	-9.539	-9.669	-0.130		
(0)							

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

Phase	SI**	log IAP	log K(313 K, 37 atm)	
Anhydrite	-0.75	-5.18	-4.43	CaSO4
Aragonite	0.11	-8.31	-8.41	CaCO3
Calcite	0.24	-8.31	-8.55	CaCO3
CH4 (g)	-23.91	-26.85	-2.93	CH4
CO2 (g)	-3.48	-5.13	-1.65	CO2
Dolomite	0.95	-16.41	-17.36	CaMg (CO3) 2

Gypsum	-0.62	-5.20	-4.58	CaSO4:2H2O
H2 (g)	-11.11	-14.26	-3.15	H2
H2O (g)	-1.14	-0.01	1.13	H2O
H2S (g)	-23.12	-31.09	-7.98	H2S
Halite	-2.54	-0.95	1.59	NaCl
O2 (g)	-56.30	-59.30	-3.00	O2
Sulfur	-17.82	-13.30	4.53	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.142 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
3\April17_SP\phreeqc\Apr17_ID=14+7+5+5+5_Measure.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
3\April17_SP\phreeqc\Apr17_ID=14+7+5+5+5_Measure.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.73
pe 4
redox pe
units mmol/kgw
density 1

```

Ca      33.82
Mg      49.45
Na      445
S(6)    11
Alkalinity 0.4 as HCO3-
Cl      572
water   1 # kg
REACTION_PRESSURE 1
61

```

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	4.000e-04	4.000e-04
Ca	3.382e-02	3.382e-02
Cl	5.720e-01	5.720e-01
Mg	4.945e-02	4.945e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

```

pH = 7.730
pe = 4.000
Specific Conductance (µS/cm, 40°C) = 67819
Density (g/cm³) = 1.01641
Volume (L) = 1.01745
Activity of water = 0.981
Ionic strength (mol/kgw) = 6.761e-01
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 3.635e-04
Total CO2 (mol/kg) = 3.635e-04
Temperature (°C) = 40.00
Electrical balance (eq) = 1.714e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.45
Iterations = 6
Total H = 1.110128e+02
Total O = 5.555132e+01

```

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

mole V Species cm ³ /mol	Molality	Activity	Log	Log	Log	-
			Molality	Activity	Gamma	
OH- 2.19	2.565e-06	1.543e-06	-5.591	-5.812	-0.221	-

H+	2.483e-08	1.862e-08	-7.605	-7.730	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(4)	3.635e-04					
HCO3-	2.395e-04	1.602e-04	-3.621	-3.795	-0.175	
27.66						
MgHCO3+	4.248e-05	2.641e-05	-4.372	-4.578	-0.206	
6.16						
CaHCO3+	2.773e-05	1.902e-05	-4.557	-4.721	-0.164	
10.44						
NaHCO3	2.236e-05	2.613e-05	-4.650	-4.583	0.068	
1.80						
CaCO3	8.432e-06	9.852e-06	-5.074	-5.006	0.068	-
14.56						
NaCO3-	8.387e-06	6.214e-06	-5.076	-5.207	-0.130	
4.11						
MgCO3	6.849e-06	8.003e-06	-5.164	-5.097	0.068	-
17.10						
CO2	5.162e-06	6.031e-06	-5.287	-5.220	0.068	
35.16						
CO3-2	2.577e-06	5.165e-07	-5.589	-6.287	-0.698	-
1.66						
(CO2)2	9.002e-13	1.052e-12	-12.046	-11.978	0.068	
70.32						
Ca	3.382e-02					
Ca+2	3.269e-02	7.865e-03	-1.486	-2.104	-0.619	-
16.46						
CaSO4	1.096e-03	1.281e-03	-2.960	-2.892	0.068	
7.96						
CaHCO3+	2.773e-05	1.902e-05	-4.557	-4.721	-0.164	
10.44						
CaCO3	8.432e-06	9.852e-06	-5.074	-5.006	0.068	-
14.56						
CaOH+	9.282e-08	6.878e-08	-7.032	-7.163	-0.130	
(0)						
CaHSO4+	2.687e-10	1.991e-10	-9.571	-9.701	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.565e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	3.645e-27					
H2	1.822e-27	2.129e-27	-26.739	-26.672	0.068	
28.59						
Mg	4.945e-02					
Mg+2	4.631e-02	1.290e-02	-1.334	-1.890	-0.555	-
20.81						
MgSO4	3.076e-03	3.594e-03	-2.512	-2.444	0.068	
6.30						
MgHCO3+	4.248e-05	2.641e-05	-4.372	-4.578	-0.206	
6.16						
MgOH+	1.282e-05	8.960e-06	-4.892	-5.048	-0.156	
(0)						
MgCO3	6.849e-06	8.003e-06	-5.164	-5.097	0.068	-
17.10						
Na	4.450e-01					

Na+	4.428e-01	3.144e-01	-0.354	-0.503	-0.149
0.05					
NaSO4-	2.122e-03	1.420e-03	-2.673	-2.848	-0.175
20.90					
NaHCO3	2.236e-05	2.613e-05	-4.650	-4.583	0.068
1.80					
NaCO3-	8.387e-06	6.214e-06	-5.076	-5.207	-0.130
4.11					
NaOH	4.151e-17	4.851e-17	-16.382	-16.314	0.068
(0)					
O(0)	6.158e-35				
O2	3.079e-35	3.598e-35	-34.512	-34.444	0.068
31.40					
S(6)	1.100e-02				
SO4-2	4.706e-03	8.229e-04	-2.327	-3.085	-0.757
19.21					
MgSO4	3.076e-03	3.594e-03	-2.512	-2.444	0.068
6.30					
NaSO4-	2.122e-03	1.420e-03	-2.673	-2.848	-0.175
20.90					
CaSO4	1.096e-03	1.281e-03	-2.960	-2.892	0.068
7.96					
HSO4-	2.842e-09	2.106e-09	-8.546	-8.677	-0.130
41.78					
CaHSO4+	2.687e-10	1.991e-10	-9.571	-9.701	-0.130
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.74	-5.19	-4.45	CaSO4
Aragonite	0.05	-8.39	-8.45	CaCO3
Calcite	0.19	-8.39	-8.58	CaCO3
CO2(g)	-3.59	-5.22	-1.63	CO2
Dolomite	0.85	-16.57	-17.42	CaMg(CO3)2
Gypsum	-0.61	-5.21	-4.60	CaSO4:2H2O
H2(g)	-23.54	-26.67	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-31.46	-34.44	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
C	3.635e-04	3.635e-04
Ca	3.382e-02	3.382e-02
Cl	5.720e-01	5.720e-01
Mg	4.945e-02	4.945e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	7.712	Charge balance
	pe =	8.903	Adjusted to redox
equilibrium			
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67820	
Density (g/cm^3)	=	1.01894	
Volume (L)	=	1.01493	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.761e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	4.000e-04	
Total CO2 (mol/kg)	=	3.635e-04	
Temperature (°C)	=	40.00	
Pressure (atm)	=	61.00	
Electrical balance (eq)	=	1.714e-02	
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.45	
Iterations	=	10	
Total H	=	1.110128e+02	
Total O	=	5.555132e+01	

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	Gamma
			Molality	Activity		
OH-	2.579e-06	1.554e-06	-5.589	-5.809	-0.220	-
2.18 H+	2.583e-08	1.939e-08	-7.588	-7.712	-0.125	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.11 C(-4)	0.000e+00					
36.68 CH4	0.000e+00	0.000e+00	-115.838	-115.770	0.068	
C(4)	3.635e-04					
HCO3-	2.379e-04	1.594e-04	-3.624	-3.798	-0.174	
27.71 MgHCO3+	4.250e-05	2.647e-05	-4.372	-4.577	-0.206	
6.34 CaHCO3+	2.775e-05	1.906e-05	-4.557	-4.720	-0.163	
10.56						

NaHCO3	2.367e-05	2.766e-05	-4.626	-4.558	0.068	
1.80						
CaCO3	8.595e-06	1.004e-05	-5.066	-4.998	0.068	-
14.15						
NaCO3-	8.461e-06	6.275e-06	-5.073	-5.202	-0.130	
4.63						
MgCO3	6.954e-06	8.126e-06	-5.158	-5.090	0.068	-
16.66						
CO2	5.036e-06	5.884e-06	-5.298	-5.230	0.068	
35.11						
CO3-2	2.620e-06	5.277e-07	-5.582	-6.278	-0.696	-
1.17						
(CO2) 2	8.568e-13	1.001e-12	-12.067	-11.999	0.068	
70.22						
Ca	3.382e-02					
Ca+2	3.269e-02	7.905e-03	-1.486	-2.102	-0.616	-
16.06						
CaSO4	1.096e-03	1.281e-03	-2.960	-2.892	0.068	
8.12						
CaHCO3+	2.775e-05	1.906e-05	-4.557	-4.720	-0.163	
10.56						
CaCO3	8.595e-06	1.004e-05	-5.066	-4.998	0.068	-
14.15						
CaOH+	8.994e-08	6.671e-08	-7.046	-7.176	-0.130	
(0)						
CaHSO4+	2.849e-10	2.113e-10	-9.545	-9.675	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.571e-01	-0.243	-0.447	-0.205	
19.09						
H(0)	5.768e-37					
H2	2.884e-37	3.370e-37	-36.540	-36.472	0.068	
28.56						
Mg	4.945e-02					
Mg+2	4.633e-02	1.296e-02	-1.334	-1.887	-0.553	-
20.36						
MgSO4	3.057e-03	3.573e-03	-2.515	-2.447	0.068	
6.46						
MgHCO3+	4.250e-05	2.647e-05	-4.372	-4.577	-0.206	
6.34						
MgOH+	1.230e-05	8.604e-06	-4.910	-5.065	-0.155	
(0)						
MgCO3	6.954e-06	8.126e-06	-5.158	-5.090	0.068	-
16.66						
Na	4.450e-01					
Na+	4.428e-01	3.148e-01	-0.354	-0.502	-0.148	
0.23						
NaSO4-	2.131e-03	1.427e-03	-2.671	-2.845	-0.174	
20.51						
NaHCO3	2.367e-05	2.766e-05	-4.626	-4.558	0.068	
1.80						
NaCO3-	8.461e-06	6.275e-06	-5.073	-5.202	-0.130	
4.63						
NaOH	4.167e-17	4.869e-17	-16.380	-16.313	0.068	
(0)						
O(0)	2.177e-15					

O2	1.088e-15	1.272e-15	-14.963	-14.896	0.068
31.28					
S(-2)	0.000e+00				
HS-	0.000e+00	0.000e+00	-112.006	-112.226	-0.220
21.90					
H2S	0.000e+00	0.000e+00	-113.248	-113.181	0.068
37.10					
S-2	0.000e+00	0.000e+00	-116.256	-116.984	-0.728
(0)					
S(6)	1.100e-02				
SO4-2	4.715e-03	8.288e-04	-2.326	-3.082	-0.755
18.96					
MgSO4	3.057e-03	3.573e-03	-2.515	-2.447	0.068
6.46					
NaSO4-	2.131e-03	1.427e-03	-2.671	-2.845	-0.174
20.51					
CaSO4	1.096e-03	1.281e-03	-2.960	-2.892	0.068
8.12					
HSO4-	2.824e-09	2.094e-09	-8.549	-8.679	-0.130
41.61					
CaHSO4+	2.849e-10	2.113e-10	-9.545	-9.675	-0.130
(0)					

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

Phase	SI**	log IAP	log K(313 K, 61 atm)	
Anhydrite	-0.78	-5.18	-4.41	CaSO4
Aragonite	0.01	-8.38	-8.39	CaCO3
Calcite	0.15	-8.38	-8.52	CaCO3
CH4(g)	-112.82	-115.77	-2.95	CH4
CO2(g)	-3.57	-5.23	-1.66	CO2
Dolomite	0.77	-16.54	-17.32	CaMg(CO3)2
Gypsum	-0.64	-5.20	-4.56	CaSO4:2H2O
H2(g)	-33.32	-36.47	-3.16	H2
H2O(g)	-1.13	-0.01	1.12	H2O
H2S(g)	-111.95	-119.94	-7.98	H2S
Halite	-2.54	-0.95	1.59	NaCl
O2(g)	-11.88	-14.90	-3.02	O2
Sulfur	-84.46	-79.95	4.51	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

 Reading input data for simulation 2.

 End of Run after 0.151 Seconds.

Input file: D:\KU\Thesis Writing\4) Results\Story
3\April17_SP\phreeqc\Apr17_ID=14+7+5+5+5_Test.pqi
Output file: D:\KU\Thesis Writing\4) Results\Story
3\April17_SP\phreeqc\Apr17_ID=14+7+5+5+5_Test.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 7.73
pe 4
redox pe
units mmol/kgw
density 1
Ca 33.82
Mg 49.45
Na 445
S(6) 11
Alkalinity 0.34 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
61

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	3.400e-04	3.400e-04
Ca	3.382e-02	3.382e-02
Cl	5.720e-01	5.720e-01

Mg	4.945e-02	4.945e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

--

	pH	=	7.730
	pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)		=	67819
Density (g/cm^3)		=	1.01640
Volume (L)		=	1.01745
Activity of water		=	0.981
Ionic strength (mol/kgw)		=	6.761e-01
Mass of water (kg)		=	1.000e+00
Total carbon (mol/kg)		=	3.068e-04
Total CO2 (mol/kg)		=	3.068e-04
Temperature (°C)		=	40.00
Electrical balance (eq)		=	1.720e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$		=	1.45
	Iterations	=	6
	Total H	=	1.110127e+02
	Total O	=	5.555115e+01

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	2.565e-06	1.543e-06	-5.591	-5.812	-0.221	-
2.19						
H+	2.483e-08	1.862e-08	-7.605	-7.730	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(4)	3.068e-04					
HCO3-	2.021e-04	1.352e-04	-3.694	-3.869	-0.175	
27.66						
MgHCO3+	3.585e-05	2.229e-05	-4.445	-4.652	-0.206	
6.16						
CaHCO3+	2.340e-05	1.605e-05	-4.631	-4.794	-0.164	
10.44						
NaHCO3	1.887e-05	2.205e-05	-4.724	-4.657	0.068	
1.80						
CaCO3	7.117e-06	8.316e-06	-5.148	-5.080	0.068	-
14.56						
NaCO3-	7.078e-06	5.244e-06	-5.150	-5.280	-0.130	
4.11						
MgCO3	5.781e-06	6.755e-06	-5.238	-5.170	0.068	-
17.10						
CO2	4.356e-06	5.090e-06	-5.361	-5.293	0.068	
35.16						
CO3-2	2.175e-06	4.359e-07	-5.663	-6.361	-0.698	-
1.66						

(CO2)2	6.411e-13	7.491e-13	-12.193	-12.125	0.068	
70.32						
Ca	3.382e-02					
Ca+2	3.269e-02	7.866e-03	-1.486	-2.104	-0.619	-
16.46						
CaSO4	1.097e-03	1.281e-03	-2.960	-2.892	0.068	
7.96						
CaHCO3+	2.340e-05	1.605e-05	-4.631	-4.794	-0.164	
10.44						
CaCO3	7.117e-06	8.316e-06	-5.148	-5.080	0.068	-
14.56						
CaOH+	9.284e-08	6.879e-08	-7.032	-7.162	-0.130	
(0)						
CaHSO4+	2.687e-10	1.991e-10	-9.571	-9.701	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.565e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	3.645e-27					
H2	1.822e-27	2.129e-27	-26.739	-26.672	0.068	
28.59						
Mg	4.945e-02					
Mg+2	4.632e-02	1.290e-02	-1.334	-1.889	-0.555	-
20.81						
MgSO4	3.076e-03	3.594e-03	-2.512	-2.444	0.068	
6.30						
MgHCO3+	3.585e-05	2.229e-05	-4.445	-4.652	-0.206	
6.16						
MgOH+	1.282e-05	8.961e-06	-4.892	-5.048	-0.156	
(0)						
MgCO3	5.781e-06	6.755e-06	-5.238	-5.170	0.068	-
17.10						
Na	4.450e-01					
Na+	4.429e-01	3.144e-01	-0.354	-0.503	-0.149	
0.05						
NaSO4-	2.122e-03	1.420e-03	-2.673	-2.848	-0.175	
20.90						
NaHCO3	1.887e-05	2.205e-05	-4.724	-4.657	0.068	
1.80						
NaCO3-	7.078e-06	5.244e-06	-5.150	-5.280	-0.130	
4.11						
NaOH	4.152e-17	4.851e-17	-16.382	-16.314	0.068	
(0)						
O(0)	6.158e-35					
O2	3.079e-35	3.598e-35	-34.512	-34.444	0.068	
31.40						
S(6)	1.100e-02					
SO4-2	4.706e-03	8.229e-04	-2.327	-3.085	-0.757	
19.21						
MgSO4	3.076e-03	3.594e-03	-2.512	-2.444	0.068	
6.30						
NaSO4-	2.122e-03	1.420e-03	-2.673	-2.848	-0.175	
20.90						
CaSO4	1.097e-03	1.281e-03	-2.960	-2.892	0.068	
7.96						
HSO4-	2.841e-09	2.105e-09	-8.546	-8.677	-0.130	
41.78						

CaHSO4+ 2.687e-10 1.991e-10 -9.571 -9.701 -0.130
 (0)

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

--

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.74	-5.19	-4.45	CaSO4
Aragonite	-0.02	-8.46	-8.45	CaCO3
Calcite	0.11	-8.46	-8.58	CaCO3
CO2(g)	-3.67	-5.29	-1.63	CO2
Dolomite	0.71	-16.71	-17.42	CaMg(CO3)2
Gypsum	-0.61	-5.21	-4.60	CaSO4:2H2O
H2(g)	-23.54	-26.67	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-31.46	-34.44	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.

Using pressure 1.

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

--

Elements	Molality	Moles
C	3.068e-04	3.068e-04
Ca	3.382e-02	3.382e-02
Cl	5.720e-01	5.720e-01
Mg	4.945e-02	4.945e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	7.713	Charge balance
	pe =	-2.425	Adjusted to redox
equilibrium			
Specific Conductance (µS/cm, 40°C)	=	67820	
Density (g/cm³)	=	1.01894	
Volume (L)	=	1.01492	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.761e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	3.400e-04	
Total CO2 (mol/kg)	=	3.068e-04	

Temperature (°C) = 40.00
 Pressure (atm) = 61.00
 Electrical balance (eq) = 1.720e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.45
 Iterations = 13
 Total H = 1.110127e+02
 Total O = 5.555115e+01

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

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm ³ /mol						
OH-	2.584e-06	1.557e-06	-5.588	-5.808	-0.220	-
2.18						
H+	2.578e-08	1.935e-08	-7.589	-7.713	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.11						
C(-4)	5.137e-26					
CH4	5.137e-26	6.002e-26	-25.289	-25.222	0.068	
36.68						
C(4)	3.068e-04					
HCO3-	2.007e-04	1.345e-04	-3.697	-3.871	-0.174	
27.71						
MgHCO3+	3.587e-05	2.234e-05	-4.445	-4.651	-0.206	
6.34						
CaHCO3+	2.342e-05	1.608e-05	-4.630	-4.794	-0.163	
10.56						
NaHCO3	1.998e-05	2.334e-05	-4.700	-4.632	0.068	
1.80						
CaCO3	7.269e-06	8.493e-06	-5.139	-5.071	0.068	-
14.15						
NaCO3-	7.154e-06	5.306e-06	-5.145	-5.275	-0.130	
4.63						
MgCO3	5.881e-06	6.872e-06	-5.231	-5.163	0.068	-
16.66						
CO2	4.241e-06	4.956e-06	-5.373	-5.305	0.068	
35.11						
CO3-2	2.215e-06	4.462e-07	-5.655	-6.351	-0.696	-
1.17						
(CO2)2	6.077e-13	7.101e-13	-12.216	-12.149	0.068	
70.22						
Ca	3.382e-02					
Ca+2	3.269e-02	7.906e-03	-1.486	-2.102	-0.616	-
16.06						
CaSO4	1.097e-03	1.281e-03	-2.960	-2.892	0.068	
8.12						
CaHCO3+	2.342e-05	1.608e-05	-4.630	-4.794	-0.163	
10.56						
CaCO3	7.269e-06	8.493e-06	-5.139	-5.071	0.068	-
14.15						
CaOH+	9.013e-08	6.685e-08	-7.045	-7.175	-0.130	
(0)						

CaHSO4+	2.843e-10	2.109e-10	-9.546	-9.676	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.571e-01	-0.243	-0.447	-0.205	
19.09						
H(0)	2.611e-14					
H2	1.305e-14	1.525e-14	-13.884	-13.817	0.068	
28.56						
Mg	4.945e-02					
Mg+2	4.634e-02	1.297e-02	-1.334	-1.887	-0.553	-
20.36						
MgSO4	3.058e-03	3.573e-03	-2.515	-2.447	0.068	
6.46						
MgHCO3+	3.587e-05	2.234e-05	-4.445	-4.651	-0.206	
6.34						
MgOH+	1.233e-05	8.623e-06	-4.909	-5.064	-0.155	
(0)						
MgCO3	5.881e-06	6.872e-06	-5.231	-5.163	0.068	-
16.66						
Na	4.450e-01					
Na+	4.428e-01	3.148e-01	-0.354	-0.502	-0.148	
0.23						
NaSO4-	2.131e-03	1.427e-03	-2.672	-2.845	-0.174	
20.51						
NaHCO3	1.998e-05	2.334e-05	-4.700	-4.632	0.068	
1.80						
NaCO3-	7.154e-06	5.306e-06	-5.145	-5.275	-0.130	
4.63						
NaOH	4.175e-17	4.879e-17	-16.379	-16.312	0.068	
(0)						
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-60.275	-60.207	0.068	
31.28						
S(-2)	4.371e-22					
HS-	4.135e-22	2.491e-22	-21.384	-21.604	-0.220	
21.90						
H2S	2.360e-23	2.757e-23	-22.627	-22.560	0.068	
37.10						
S-2	2.327e-26	4.352e-27	-25.633	-26.361	-0.728	
(0)						
S(6)	1.100e-02					
SO4-2	4.715e-03	8.287e-04	-2.327	-3.082	-0.755	
18.96						
MgSO4	3.058e-03	3.573e-03	-2.515	-2.447	0.068	
6.46						
NaSO4-	2.131e-03	1.427e-03	-2.672	-2.845	-0.174	
20.51						
CaSO4	1.097e-03	1.281e-03	-2.960	-2.892	0.068	
8.12						
HSO4-	2.818e-09	2.090e-09	-8.550	-8.680	-0.130	
41.61						
CaHSO4+	2.843e-10	2.109e-10	-9.546	-9.676	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K, 61 atm)	
Anhydrite	-0.78	-5.18	-4.41	CaSO4
Aragonite	-0.06	-8.45	-8.39	CaCO3
Calcite	0.07	-8.45	-8.52	CaCO3
CH4(g)	-22.27	-25.22	-2.95	CH4
CO2(g)	-3.64	-5.30	-1.66	CO2
Dolomite	0.63	-16.69	-17.32	CaMg(CO3)2
Gypsum	-0.64	-5.20	-4.56	CaSO4:2H2O
H2(g)	-10.66	-13.82	-3.16	H2
H2O(g)	-1.13	-0.01	1.12	H2O
H2S(g)	-21.33	-29.32	-7.98	H2S
Halite	-2.54	-0.95	1.59	NaCl
O2(g)	-57.19	-60.21	-3.02	O2
Sulfur	-16.49	-11.98	4.51	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.155 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\T=40.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\T=40.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

```

SOLUTION 1
  temp      40
  pH        8.2
  pe        4
  redox     pe
  units     mmol/kgw
  density   1
  Ca        35
  Mg        48
  Na        445
  S(6)     11
  Alkalinity 2.4 as HCO3-
  Cl        572
  water     1 # kgw

```

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

```

pH = 8.200
pe = 4.000
Specific Conductance (µS/cm, 40°C) = 67832
Density (g/cm³) = 1.01647
Volume (L) = 1.01750
Activity of water = 0.981
Ionic strength (mol/kgw) = 6.753e-01
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 1.989e-03
Total CO2 (mol/kg) = 1.989e-03
Temperature (°C) = 40.00
Electrical balance (eq) = 1.460e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
Iterations = 7
Total H = 1.110141e+02
Total O = 5.555622e+01

```

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

```

mole V
Log      Log      Log

```

Species cm ³ /mol	Molality	Activity	Molality	Activity	Gamma	
OH- 2.19	7.568e-06	4.553e-06	-5.121	-5.342	-0.221	-
H+ 0.00	8.413e-09	6.310e-09	-8.075	-8.200	-0.125	
H2O 18.16	5.551e+01	9.812e-01	1.744	-0.008	0.000	
C (4)	1.989e-03					
HCO3- 27.66	1.160e-03	7.764e-04	-2.935	-3.110	-0.174	
MgHCO3+ 6.16	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
CaHCO3+ 10.44	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
CaCO3 14.56	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
NaCO3- 4.11	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
NaHCO3 1.80	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
MgCO3 17.10	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
CO3-2 1.66	3.684e-05	7.386e-06	-4.434	-5.132	-0.698	-
CO2 35.16	8.476e-06	9.902e-06	-5.072	-5.004	0.068	
(CO2) 2 70.32	2.427e-12	2.835e-12	-11.615	-11.547	0.068	
Ca	3.500e-02					
Ca+2 16.46	3.360e-02	8.086e-03	-1.474	-2.092	-0.619	-
CaSO4 7.96	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
CaHCO3+ 10.44	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
CaCO3 14.56	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
CaOH+ (0)	2.817e-07	2.087e-07	-6.550	-6.681	-0.130	
CaHSO4+ (0)	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
Cl	5.720e-01					
Cl- 19.08	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
H (0)	4.185e-28					
H2 28.59	2.093e-28	2.445e-28	-27.679	-27.612	0.068	
Mg	4.800e-02					
Mg+2 20.81	4.468e-02	1.244e-02	-1.350	-1.905	-0.555	-
MgSO4 6.30	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
MgHCO3+ 6.16	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	

MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
MgOH+	3.650e-05	2.551e-05	-4.438	-4.593	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.142e-01	-0.354	-0.503	-0.149	
0.05						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
NaOH	1.225e-16	1.431e-16	-15.912	-15.844	0.068	
(0)						
O(0)	4.672e-33					
O2	2.336e-33	2.729e-33	-32.632	-32.564	0.068	
31.40						
S(6)	1.100e-02					
SO4-2	4.738e-03	8.290e-04	-2.324	-3.081	-0.757	
19.21						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
HSO4-	9.700e-10	7.187e-10	-9.013	-9.143	-0.130	
41.78						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.72	-5.17	-4.45	CaSO4
Aragonite	1.22	-7.22	-8.45	CaCO3
Calcite	1.36	-7.22	-8.58	CaCO3
CO2(g)	-3.38	-5.00	-1.63	CO2
Dolomite	3.16	-14.26	-17.42	CaMg(CO3)2
Gypsum	-0.59	-5.19	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-29.58	-32.56	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

 Reading input data for simulation 2.

End of Run after 0.394 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 1atm, T variable\T=42.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 1atm, T variable\T=42.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 42
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kgw

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
----------	----------	-------

Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance (μS/cm, 42°C)	=	70069
Density (g/cm³)	=	1.01565
Volume (L)	=	1.01832
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.751e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.963e-03
Total CO2 (mol/kg)	=	1.963e-03
Temperature (°C)	=	42.00
Electrical balance (eq)	=	1.460e-02
Percent error, 100*(Cat- An)/(Cat+ An)	=	1.23
Iterations	=	7
Total H	=	1.110140e+02
Total O	=	5.555615e+01

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

mole V Species cm³/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	8.634e-06	5.186e-06	-5.064	-5.285	-0.221	-
2.17						
H+	8.420e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.17						
C(4)	1.963e-03					
HCO3-	1.127e-03	7.534e-04	-2.948	-3.123	-0.175	
27.71						
MgHCO3+	1.945e-04	1.208e-04	-3.711	-3.918	-0.207	
6.19						
CaHCO3+	1.355e-04	9.285e-05	-3.868	-4.032	-0.164	
10.49						
NaCO3-	1.306e-04	9.662e-05	-3.884	-4.015	-0.131	
4.21						
CaCO3	1.299e-04	1.517e-04	-3.886	-3.819	0.068	-
14.55						
NaHCO3	1.039e-04	1.214e-04	-3.983	-3.916	0.068	
1.80						
MgCO3	9.631e-05	1.125e-04	-4.016	-3.949	0.068	-
17.10						

CO3-2	3.684e-05	7.349e-06	-4.434	-5.134	-0.700	-
1.70						
CO2	8.154e-06	9.526e-06	-5.089	-5.021	0.068	
35.26						
(CO2)2	2.372e-12	2.771e-12	-11.625	-11.557	0.068	
70.52						
Ca	3.500e-02					
Ca+2	3.361e-02	8.043e-03	-1.474	-2.095	-0.621	-
16.44						
CaSO4	1.127e-03	1.316e-03	-2.948	-2.881	0.068	
8.01						
CaHCO3+	1.355e-04	9.285e-05	-3.868	-4.032	-0.164	
10.49						
CaCO3	1.299e-04	1.517e-04	-3.886	-3.819	0.068	-
14.55						
CaOH+	2.805e-07	2.076e-07	-6.552	-6.683	-0.131	
(0)						
CaHSO4+	9.702e-11	7.180e-11	-10.013	-10.144	-0.131	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.560e-01	-0.243	-0.449	-0.206	
19.09						
H(0)	4.111e-28					
H2	2.056e-28	2.401e-28	-27.687	-27.620	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.461e-02	1.236e-02	-1.351	-1.908	-0.557	-
20.86						
MgSO4	3.061e-03	3.576e-03	-2.514	-2.447	0.068	
6.35						
MgHCO3+	1.945e-04	1.208e-04	-3.711	-3.918	-0.207	
6.19						
MgCO3	9.631e-05	1.125e-04	-4.016	-3.949	0.068	-
17.10						
MgOH+	4.271e-05	2.981e-05	-4.369	-4.526	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.138e-01	-0.354	-0.503	-0.149	
0.11						
NaSO4-	2.125e-03	1.420e-03	-2.673	-2.848	-0.175	
20.82						
NaCO3-	1.306e-04	9.662e-05	-3.884	-4.015	-0.131	
4.21						
NaHCO3	1.039e-04	1.214e-04	-3.983	-3.916	0.068	
1.80						
NaOH	1.393e-16	1.627e-16	-15.856	-15.789	0.068	
(0)						
O(0)	1.847e-32					
O2	9.236e-33	1.079e-32	-32.035	-31.967	0.068	
31.51						
S(6)	1.100e-02					
SO4-2	4.687e-03	8.157e-04	-2.329	-3.088	-0.759	
19.36						
MgSO4	3.061e-03	3.576e-03	-2.514	-2.447	0.068	
6.35						
NaSO4-	2.125e-03	1.420e-03	-2.673	-2.848	-0.175	
20.82						

CaSO4	1.127e-03	1.316e-03	-2.948	-2.881	0.068
8.01					
HSO4-	1.003e-09	7.425e-10	-8.999	-9.129	-0.131
41.86					
CaHSO4+	9.702e-11	7.180e-11	-10.013	-10.144	-0.131
(0)					

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

Phase	SI**	log IAP	log K(315 K,	1 atm)
Anhydrite	-0.71	-5.18	-4.48	CaSO4
Aragonite	1.23	-7.23	-8.46	CaCO3
Calcite	1.37	-7.23	-8.60	CaCO3
CO2(g)	-3.38	-5.02	-1.64	CO2
Dolomite	3.19	-14.27	-17.46	CaMg(CO3)2
Gypsum	-0.60	-5.20	-4.60	CaSO4:2H2O
H2(g)	-24.49	-27.62	-3.13	H2
H2O(g)	-1.10	-0.01	1.09	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-28.97	-31.97	-2.99	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.116 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\T=45.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\T=45.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 45
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 45°C)	=	73449
Density (g/cm^3)	=	1.01436
Volume (L)	=	1.01961
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.747e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.922e-03
Total CO2 (mol/kg)	=	1.922e-03
Temperature (°C)	=	45.00
Electrical balance (eq)	=	1.460e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23
Iterations	=	7

Total H = 1.110140e+02

Total O = 5.555604e+01

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

--

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.047e-05	6.273e-06	-4.980	-5.202	-0.222	-
2.14						
H+	8.431e-09	6.310e-09	-8.074	-8.200	-0.126	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.19						
C(4)	1.922e-03					
HCO3-	1.077e-03	7.181e-04	-2.968	-3.144	-0.176	
27.79						
MgHCO3+	1.883e-04	1.166e-04	-3.725	-3.933	-0.208	
6.23						
NaCO3-	1.472e-04	1.088e-04	-3.832	-3.964	-0.132	
4.34						
CaCO3	1.388e-04	1.621e-04	-3.858	-3.790	0.067	-
14.55						
CaHCO3+	1.310e-04	8.963e-05	-3.883	-4.048	-0.165	
10.56						
MgCO3	9.848e-05	1.150e-04	-4.007	-3.939	0.067	-
17.10						
NaHCO3	9.732e-05	1.137e-04	-4.012	-3.944	0.067	
1.80						
CO3-2	3.663e-05	7.250e-06	-4.436	-5.140	-0.704	-
1.80						
CO2	7.698e-06	8.992e-06	-5.114	-5.046	0.067	
35.41						
(CO2)2	2.289e-12	2.674e-12	-11.640	-11.573	0.067	
70.81						
Ca	3.500e-02					
Ca+2	3.362e-02	7.978e-03	-1.473	-2.098	-0.625	-
16.43						
CaSO4	1.113e-03	1.300e-03	-2.954	-2.886	0.067	
8.08						
CaCO3	1.388e-04	1.621e-04	-3.858	-3.790	0.067	-
14.55						
CaHCO3+	1.310e-04	8.963e-05	-3.883	-4.048	-0.165	
10.56						
CaOH+	2.788e-07	2.059e-07	-6.555	-6.686	-0.132	
(0)						
CaHSO4+	1.013e-10	7.486e-11	-9.994	-10.126	-0.132	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.551e-01	-0.243	-0.450	-0.207	
19.10						
H(0)	4.004e-28					
H2	2.002e-28	2.339e-28	-27.699	-27.631	0.067	
28.59						

Mg	4.800e-02						
Mg+2	4.449e-02	1.223e-02	-1.352	-1.913	-0.561	-	
20.95							
MgSO4	3.166e-03	3.698e-03	-2.499	-2.432	0.067		
6.42							
MgHCO3+	1.883e-04	1.166e-04	-3.725	-3.933	-0.208		
6.23							
MgCO3	9.848e-05	1.150e-04	-4.007	-3.939	0.067	-	
17.10							
MgOH+	5.383e-05	3.751e-05	-4.269	-4.426	-0.157		
(0)							
Na	4.450e-01						
Na+	4.426e-01	3.130e-01	-0.354	-0.504	-0.151		
0.19							
NaSO4-	2.109e-03	1.406e-03	-2.676	-2.852	-0.176		
20.69							
NaCO3-	1.472e-04	1.088e-04	-3.832	-3.964	-0.132		
4.34							
NaHCO3	9.732e-05	1.137e-04	-4.012	-3.944	0.067		
1.80							
NaOH	1.681e-16	1.964e-16	-15.774	-15.707	0.067		
(0)							
O(0)	1.406e-31						
O2	7.029e-32	8.210e-32	-31.153	-31.086	0.067		
31.67							
S(6)	1.100e-02						
SO4-2	4.612e-03	7.961e-04	-2.336	-3.099	-0.763		
19.56							
MgSO4	3.166e-03	3.698e-03	-2.499	-2.432	0.067		
6.42							
NaSO4-	2.109e-03	1.406e-03	-2.676	-2.852	-0.176		
20.69							
CaSO4	1.113e-03	1.300e-03	-2.954	-2.886	0.067		
8.08							
HSO4-	1.056e-09	7.804e-10	-8.976	-9.108	-0.132		
41.96							
CaHSO4+	1.013e-10	7.486e-11	-9.994	-10.126	-0.132		
(0)							

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

Phase	SI**	log IAP	log K(318 K,	1 atm)
Anhydrite	-0.68	-5.20	-4.51	CaSO4
Aragonite	1.25	-7.24	-8.49	CaCO3
Calcite	1.38	-7.24	-8.62	CaCO3
CO2(g)	-3.38	-5.05	-1.67	CO2
Dolomite	3.23	-14.29	-17.52	CaMg(CO3)2
Gypsum	-0.61	-5.21	-4.61	CaSO4:2H2O
H2(g)	-24.50	-27.63	-3.13	H2
H2O(g)	-1.03	-0.01	1.03	H2O
Halite	-2.54	-0.95	1.59	NaCl
O2(g)	-28.08	-31.09	-3.01	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.109 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 1atm, T variable\T=49.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 1atm, T variable\T=49.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 49
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

--

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

--

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 49°C)	=	77999
Density (g/cm^3)	=	1.01257
Volume (L)	=	1.02142
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.742e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.864e-03
Total CO2 (mol/kg)	=	1.864e-03
Temperature (°C)	=	49.00
Electrical balance (eq)	=	1.460e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23
Iterations	=	7
Total H	=	1.110139e+02
Total O	=	5.555589e+01

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

--

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm^3/mol						
OH-	1.343e-05	8.018e-06	-4.872	-5.096	-0.224	-
2.12						
H+	8.447e-09	6.310e-09	-8.073	-8.200	-0.127	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.23						
C(4)	1.864e-03					
HCO3-	1.007e-03	6.700e-04	-2.997	-3.174	-0.177	
27.86						
MgHCO3+	1.796e-04	1.109e-04	-3.746	-3.955	-0.209	
6.28						
NaCO3-	1.702e-04	1.254e-04	-3.769	-3.902	-0.133	
4.47						

CaCO3	1.504e-04	1.757e-04	-3.823	-3.755	0.067	-
14.54						
CaHCO3+	1.242e-04	8.475e-05	-3.906	-4.072	-0.166	
10.64						
MgCO3	1.003e-04	1.171e-04	-3.999	-3.931	0.067	-
17.10						
NaHCO3	8.875e-05	1.037e-04	-4.052	-3.984	0.067	
1.80						
CO3-2	3.597e-05	7.042e-06	-4.444	-5.152	-0.708	-
1.99						
CO2	7.130e-06	8.327e-06	-5.147	-5.080	0.067	
35.61						
(CO2) 2	2.174e-12	2.540e-12	-11.663	-11.595	0.067	
71.22						
Ca	3.500e-02					
Ca+2	3.363e-02	7.891e-03	-1.473	-2.103	-0.630	-
16.42						
CaSO4	1.094e-03	1.278e-03	-2.961	-2.894	0.067	
8.17						
CaCO3	1.504e-04	1.757e-04	-3.823	-3.755	0.067	-
14.54						
CaHCO3+	1.242e-04	8.475e-05	-3.906	-4.072	-0.166	
10.64						
CaOH+	2.764e-07	2.036e-07	-6.558	-6.691	-0.133	
(0)						
CaHSO4+	1.076e-10	7.927e-11	-9.968	-10.101	-0.133	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.539e-01	-0.243	-0.451	-0.209	
19.10						
H(0)	3.869e-28					
H2	1.934e-28	2.259e-28	-27.713	-27.646	0.067	
28.59						
Mg	4.800e-02					
Mg+2	4.434e-02	1.206e-02	-1.353	-1.919	-0.566	-
21.06						
MgSO4	3.305e-03	3.860e-03	-2.481	-2.413	0.067	
6.51						
MgHCO3+	1.796e-04	1.109e-04	-3.746	-3.955	-0.209	
6.28						
MgCO3	1.003e-04	1.171e-04	-3.999	-3.931	0.067	-
17.10						
MgOH+	7.277e-05	5.059e-05	-4.138	-4.296	-0.158	
(0)						
Na	4.450e-01					
Na+	4.427e-01	3.120e-01	-0.354	-0.506	-0.152	
0.30						
NaSO4-	2.086e-03	1.387e-03	-2.681	-2.858	-0.177	
20.50						
NaCO3-	1.702e-04	1.254e-04	-3.769	-3.902	-0.133	
4.47						
NaHCO3	8.875e-05	1.037e-04	-4.052	-3.984	0.067	
1.80						
NaOH	2.142e-16	2.501e-16	-15.669	-15.602	0.067	
(0)						
O(0)	1.984e-30					

O2	9.921e-31	1.159e-30	-30.003	-29.936	0.067
31.88					
S(6)	1.100e-02				
SO4-2	4.516e-03	7.707e-04	-2.345	-3.113	-0.768
19.78					
MgSO4	3.305e-03	3.860e-03	-2.481	-2.413	0.067
6.51					
NaSO4-	2.086e-03	1.387e-03	-2.681	-2.858	-0.177
20.50					
CaSO4	1.094e-03	1.278e-03	-2.961	-2.894	0.067
8.17					
HSO4-	1.134e-09	8.355e-10	-8.945	-9.078	-0.133
42.08					
CaHSO4+	1.076e-10	7.927e-11	-9.968	-10.101	-0.133
(0)					

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

Phase	SI**	log IAP	log K(322 K,	1 atm)
Anhydrite	-0.65	-5.22	-4.56	CaSO4
Aragonite	1.27	-7.26	-8.53	CaCO3
Calcite	1.40	-7.26	-8.65	CaCO3
CO2(g)	-3.38	-5.08	-1.70	CO2
Dolomite	3.28	-14.33	-17.61	CaMg(CO3)2
Gypsum	-0.62	-5.23	-4.62	CaSO4:2H2O
H2(g)	-24.51	-27.65	-3.14	H2
H2O(g)	-0.95	-0.01	0.94	H2O
Halite	-2.54	-0.96	1.59	NaCl
O2(g)	-26.91	-29.94	-3.03	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.119 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\T=50.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\T=50.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 50
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kgw

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH = 8.200
pe = 4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 50°C) = 79144
Density (g/cm^3) = 1.01210
Volume (L) = 1.02188

Activity of water = 0.981
 Ionic strength (mol/kgw) = 6.741e-01
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 1.849e-03
 Total CO2 (mol/kg) = 1.849e-03
 Temperature (°C) = 50.00
 Electrical balance (eq) = 1.460e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
 Iterations = 7
 Total H = 1.110139e+02
 Total O = 5.555585e+01

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

mole V			Log	Log	Log		
Species	Molality	Activity	Molality	Activity	Gamma		
cm ³ /mol							
2.12	OH-	1.427e-05	8.512e-06	-4.846	-5.070	-0.224	-
0.00	H+	8.451e-09	6.310e-09	-8.073	-8.200	-0.127	
18.23	H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
C(4)	1.849e-03						
27.88	HCO3-	9.895e-04	6.578e-04	-3.005	-3.182	-0.177	
6.29	MgHCO3+	1.774e-04	1.094e-04	-3.751	-3.961	-0.210	
4.50	NaCO3-	1.760e-04	1.296e-04	-3.754	-3.887	-0.133	
14.53	CaCO3	1.533e-04	1.790e-04	-3.815	-3.747	0.067	-
10.66	CaHCO3+	1.224e-04	8.344e-05	-3.912	-4.079	-0.166	
17.10	MgCO3	1.005e-04	1.174e-04	-3.998	-3.930	0.067	-
1.80	NaHCO3	8.664e-05	1.012e-04	-4.062	-3.995	0.067	
2.05	CO3-2	3.573e-05	6.977e-06	-4.447	-5.156	-0.709	-
35.66	CO2	6.994e-06	8.168e-06	-5.155	-5.088	0.067	
71.32	(CO2)2	2.145e-12	2.505e-12	-11.669	-11.601	0.067	
Ca	3.500e-02						
16.41	Ca+2	3.364e-02	7.869e-03	-1.473	-2.104	-0.631	-
8.19	CaSO4	1.089e-03	1.272e-03	-2.963	-2.896	0.067	
14.53	CaCO3	1.533e-04	1.790e-04	-3.815	-3.747	0.067	-
10.66	CaHCO3+	1.224e-04	8.344e-05	-3.912	-4.079	-0.166	

CaOH+	2.758e-07	2.031e-07	-6.559	-6.692	-0.133	
(0)						
CaHSO4+	1.092e-10	8.043e-11	-9.962	-10.095	-0.133	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.536e-01	-0.243	-0.452	-0.209	
19.10						
H(0)	3.836e-28					
H2	1.918e-28	2.240e-28	-27.717	-27.650	0.067	
28.59						
Mg	4.800e-02					
Mg+2	4.430e-02	1.201e-02	-1.354	-1.920	-0.567	-
21.09						
MgSO4	3.339e-03	3.900e-03	-2.476	-2.409	0.067	
6.53						
MgHCO3+	1.774e-04	1.094e-04	-3.751	-3.961	-0.210	
6.29						
MgCO3	1.005e-04	1.174e-04	-3.998	-3.930	0.067	-
17.10						
MgOH+	7.837e-05	5.445e-05	-4.106	-4.264	-0.158	
(0)						
Na	4.450e-01					
Na+	4.427e-01	3.117e-01	-0.354	-0.506	-0.152	
0.32						
NaSO4-	2.080e-03	1.382e-03	-2.682	-2.859	-0.177	
20.45						
NaCO3-	1.760e-04	1.296e-04	-3.754	-3.887	-0.133	
4.50						
NaHCO3	8.664e-05	1.012e-04	-4.062	-3.995	0.067	
1.80						
NaOH	2.272e-16	2.653e-16	-15.644	-15.576	0.067	
(0)						
O(0)	3.807e-30					
O2	1.903e-30	2.223e-30	-29.720	-29.653	0.067	
31.92						
S(6)	1.100e-02					
SO4-2	4.492e-03	7.645e-04	-2.348	-3.117	-0.769	
19.83						
MgSO4	3.339e-03	3.900e-03	-2.476	-2.409	0.067	
6.53						
NaSO4-	2.080e-03	1.382e-03	-2.682	-2.859	-0.177	
20.45						
CaSO4	1.089e-03	1.272e-03	-2.963	-2.896	0.067	
8.19						
HSO4-	1.155e-09	8.502e-10	-8.938	-9.070	-0.133	
42.11						
CaHSO4+	1.092e-10	8.043e-11	-9.962	-10.095	-0.133	
(0)						

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

Phase	SI**	log IAP	log K(323 K,	1 atm)
Anhydrite	-0.65	-5.22	-4.58	CaSO4
Aragonite	1.28	-7.26	-8.54	CaCO3
Calcite	1.40	-7.26	-8.66	CaCO3

CO2(g)	-3.38	-5.09	-1.71	CO2
Dolomite	3.29	-14.34	-17.63	CaMg(CO3)2
Gypsum	-0.62	-5.24	-4.62	CaSO4:2H2O
H2(g)	-24.51	-27.65	-3.14	H2
H2O(g)	-0.92	-0.01	0.92	H2O
Halite	-2.55	-0.96	1.59	NaCl
O2(g)	-26.62	-29.65	-3.03	O2

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.378 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 1atm, T variable\T=55.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 1atm, T variable\T=55.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 55
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1

```

Ca      35
Mg      48
Na     445
S(6)   11
Alkalinity 2.4 as HCO3-
Cl     572
water  1 # kgg

```

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

```

pH = 8.200
pe = 4.000
Specific Conductance (µS/cm, 55°C) = 84902
Density (g/cm³) = 1.00970
Volume (L) = 1.02431
Activity of water = 0.981
Ionic strength (mol/kgw) = 6.735e-01
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 1.768e-03
Total CO2 (mol/kg) = 1.768e-03
Temperature (°C) = 55.00
Electrical balance (eq) = 1.460e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
Iterations = 8
Total H = 1.110138e+02
Total O = 5.555565e+01

```

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

mole V Species cm ³ /mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	1.917e-05	1.138e-05	-4.717	-4.944	-0.226	-
2.14 H+	8.472e-09	6.310e-09	-8.072	-8.200	-0.128	
0.00						

H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.28						
C(4)	1.768e-03					
HCO3-	9.003e-04	5.963e-04	-3.046	-3.224	-0.179	
27.94						
NaCO3-	2.050e-04	1.504e-04	-3.688	-3.823	-0.134	
4.60						
CaCO3	1.666e-04	1.946e-04	-3.778	-3.711	0.067	-
14.52						
MgHCO3+	1.660e-04	1.020e-04	-3.780	-3.992	-0.212	
6.33						
CaHCO3+	1.126e-04	7.653e-05	-3.948	-4.116	-0.168	
10.75						
MgCO3	1.006e-04	1.174e-04	-3.998	-3.930	0.067	-
17.10						
NaHCO3	7.639e-05	8.921e-05	-4.117	-4.050	0.067	
1.80						
CO3-2	3.418e-05	6.582e-06	-4.466	-5.182	-0.715	-
2.40						
CO2	6.347e-06	7.412e-06	-5.197	-5.130	0.067	
35.92						
(CO2)2	1.990e-12	2.324e-12	-11.701	-11.634	0.067	
71.84						
Ca	3.500e-02					
Ca+2	3.366e-02	7.756e-03	-1.473	-2.110	-0.637	-
16.42						
CaSO4	1.064e-03	1.242e-03	-2.973	-2.906	0.067	
8.29						
CaCO3	1.666e-04	1.946e-04	-3.778	-3.711	0.067	-
14.52						
CaHCO3+	1.126e-04	7.653e-05	-3.948	-4.116	-0.168	
10.75						
CaOH+	2.727e-07	2.002e-07	-6.564	-6.699	-0.134	
(0)						
CaHSO4+	1.181e-10	8.666e-11	-9.928	-10.062	-0.134	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.520e-01	-0.243	-0.453	-0.211	
19.06						
H(0)	3.680e-28					
H2	1.840e-28	2.148e-28	-27.735	-27.668	0.067	
28.58						
Mg	4.800e-02					
Mg+2	4.411e-02	1.179e-02	-1.355	-1.928	-0.573	-
21.23						
MgSO4	3.508e-03	4.096e-03	-2.455	-2.388	0.067	
6.63						
MgHCO3+	1.660e-04	1.020e-04	-3.780	-3.992	-0.212	
6.33						
MgOH+	1.127e-04	7.804e-05	-3.948	-4.108	-0.159	
(0)						
MgCO3	1.006e-04	1.174e-04	-3.998	-3.930	0.067	-
17.10						
Na	4.450e-01					
Na+	4.427e-01	3.104e-01	-0.354	-0.508	-0.154	
0.43						

NaSO4-	2.050e-03	1.358e-03	-2.688	-2.867	-0.179
20.15					
NaCO3-	2.050e-04	1.504e-04	-3.688	-3.823	-0.134
4.60					
NaHCO3	7.639e-05	8.921e-05	-4.117	-4.050	0.067
1.80					
NaOH	3.026e-16	3.533e-16	-15.519	-15.452	0.067
(0)					
O(0)	9.323e-29				
O2	4.662e-29	5.444e-29	-28.331	-28.264	0.067
32.16					
S(6)	1.100e-02				
SO4-2	4.379e-03	7.343e-04	-2.359	-3.134	-0.775
20.02					
MgSO4	3.508e-03	4.096e-03	-2.455	-2.388	0.067
6.63					
NaSO4-	2.050e-03	1.358e-03	-2.688	-2.867	-0.179
20.15					
CaSO4	1.064e-03	1.242e-03	-2.973	-2.906	0.067
8.29					
HSO4-	1.266e-09	9.293e-10	-8.898	-9.032	-0.134
42.23					
CaHSO4+	1.181e-10	8.666e-11	-9.928	-10.062	-0.134
(0)					

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

Phase	SI**	log IAP	log K(328 K,	1 atm)
Anhydrite	-0.60	-5.24	-4.64	CaSO4
Aragonite	1.29	-7.29	-8.59	CaCO3
Calcite	1.42	-7.29	-8.71	CaCO3
CO2(g)	-3.38	-5.13	-1.75	CO2
Dolomite	3.32	-14.40	-17.72	CaMg(CO3)2
Gypsum	-0.63	-5.26	-4.63	CaSO4:2H2O
H2(g)	-24.53	-27.67	-3.14	H2
H2O(g)	-0.82	-0.01	0.81	H2O
Halite	-2.55	-0.96	1.59	NaCl
O2(g)	-25.22	-28.26	-3.05	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

 Reading input data for simulation 2.

 End of Run after 0.113 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 1atm, T variable\T=60.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 1atm, T variable\T=60.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 60
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH = 8.200
 pe = 4.000
 Specific Conductance ($\mu\text{S}/\text{cm}$, 60°C) = 90709
 Density (g/cm^3) = 1.00716
 Volume (L) = 1.02689
 Activity of water = 0.981
 Ionic strength (mol/kgw) = $6.729\text{e-}01$
 Mass of water (kg) = $1.000\text{e+}00$
 Total carbon (mol/kg) = $1.679\text{e-}03$
 Total CO2 (mol/kg) = $1.679\text{e-}03$
 Temperature ($^\circ\text{C}$) = 60.00
 Electrical balance (eq) = $1.460\text{e-}02$
 Percent error, $100 * (\text{Cat-}|\text{An}|) / (\text{Cat+}|\text{An}|)$ = 1.24
 Iterations = 8
 Total H = $1.110138\text{e+}02$
 Total O = $5.555543\text{e+}01$

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

mole V Species cm^3/mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	$2.541\text{e-}05$	$1.501\text{e-}05$	-4.595	-4.824	-0.228	-
2.18 H+	$8.493\text{e-}09$	$6.310\text{e-}09$	-8.071	-8.200	-0.129	
0.00 H2O	$5.551\text{e+}01$	$9.812\text{e-}01$	1.744	-0.008	0.000	
18.32 C(4)	$1.679\text{e-}03$					
HCO3-	$8.099\text{e-}04$	$5.345\text{e-}04$	-3.092	-3.272	-0.180	
27.97 NaCO3-	$2.323\text{e-}04$	$1.699\text{e-}04$	-3.634	-3.770	-0.136	
4.64 CaCO3	$1.780\text{e-}04$	$2.078\text{e-}04$	-3.750	-3.682	0.067	-
14.51 MgHCO3+	$1.540\text{e-}04$	$9.418\text{e-}05$	-3.813	-4.026	-0.214	
6.36 CaHCO3+	$1.022\text{e-}04$	$6.921\text{e-}05$	-3.991	-4.160	-0.169	
10.82 MgCO3	$9.846\text{e-}05$	$1.150\text{e-}04$	-4.007	-3.939	0.067	-
17.09 NaHCO3	$6.663\text{e-}05$	$7.779\text{e-}05$	-4.176	-4.109	0.067	
1.80 CO3-2	$3.206\text{e-}05$	$6.084\text{e-}06$	-4.494	-5.216	-0.722	-
2.84 CO2	$5.744\text{e-}06$	$6.707\text{e-}06$	-5.241	-5.173	0.067	
36.19 (CO2)2	$1.822\text{e-}12$	$2.128\text{e-}12$	-11.739	-11.672	0.067	
72.38 Ca	$3.500\text{e-}02$					

Ca+2	3.368e-02	7.642e-03	-1.473	-2.117	-0.644	-
16.44						
CaSO4	1.038e-03	1.212e-03	-2.984	-2.916	0.067	
8.37						
CaCO3	1.780e-04	2.078e-04	-3.750	-3.682	0.067	-
14.51						
CaHCO3+	1.022e-04	6.921e-05	-3.991	-4.160	-0.169	
10.82						
CaOH+	2.696e-07	1.972e-07	-6.569	-6.705	-0.136	
(0)						
CaHSO4+	1.280e-10	9.361e-11	-9.893	-10.029	-0.136	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.503e-01	-0.243	-0.456	-0.213	
19.00						
H(0)	3.534e-28					
H2	1.767e-28	2.063e-28	-27.753	-27.685	0.067	
28.58						
Mg	4.800e-02					
Mg+2	4.392e-02	1.157e-02	-1.357	-1.937	-0.579	-
21.38						
MgSO4	3.671e-03	4.286e-03	-2.435	-2.368	0.067	
6.72						
MgOH+	1.601e-04	1.105e-04	-3.796	-3.957	-0.161	
(0)						
MgHCO3+	1.540e-04	9.418e-05	-3.813	-4.026	-0.214	
6.36						
MgCO3	9.846e-05	1.150e-04	-4.007	-3.939	0.067	-
17.09						
Na	4.450e-01					
Na+	4.427e-01	3.090e-01	-0.354	-0.510	-0.156	
0.54						
NaSO4-	2.019e-03	1.332e-03	-2.695	-2.875	-0.180	
19.82						
NaCO3-	2.323e-04	1.699e-04	-3.634	-3.770	-0.136	
4.64						
NaHCO3	6.663e-05	7.779e-05	-4.176	-4.109	0.067	
1.80						
NaOH	3.973e-16	4.639e-16	-15.401	-15.334	0.067	
(0)						
O(0)	2.074e-27					
O2	1.037e-27	1.211e-27	-26.984	-26.917	0.067	
32.38						
S(6)	1.100e-02					
SO4-2	4.271e-03	7.054e-04	-2.369	-3.152	-0.782	
20.15						
MgSO4	3.671e-03	4.286e-03	-2.435	-2.368	0.067	
6.72						
NaSO4-	2.019e-03	1.332e-03	-2.695	-2.875	-0.180	
19.82						
CaSO4	1.038e-03	1.212e-03	-2.984	-2.916	0.067	
8.37						
HSO4-	1.393e-09	1.019e-09	-8.856	-8.992	-0.136	
42.31						
CaHSO4+	1.280e-10	9.361e-11	-9.893	-10.029	-0.136	
(0)						

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

--

Phase	SI**	log IAP	log K(333 K,	1 atm)
Anhydrite	-0.56	-5.27	-4.71	CaSO4
Aragonite	1.30	-7.33	-8.64	CaCO3
Calcite	1.43	-7.33	-8.76	CaCO3
CO2(g)	-3.39	-5.17	-1.78	CO2
Dolomite	3.33	-14.49	-17.82	CaMg(CO3)2
Gypsum	-0.63	-5.28	-4.65	CaSO4:2H2O
H2(g)	-24.55	-27.69	-3.14	H2
H2O(g)	-0.72	-0.01	0.71	H2O
Halite	-2.56	-0.97	1.60	NaCl
O2(g)	-23.85	-26.92	-3.06	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.114 Seconds.

Input file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\P =
1atm, T variable\T=65.pqi
Output file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\P =
1atm, T variable\T=65.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 65
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 65°C)	=	96553
Density (g/cm^3)	=	1.00448
Volume (L)	=	1.02962
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.723e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.581e-03
Total CO2 (mol/kg)	=	1.581e-03
Temperature (°C)	=	65.00
Electrical balance (eq)	=	1.460e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.24
Iterations	=	8
Total H	=	1.110137e+02
Total O	=	5.555521e+01

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

mole V Species cm ³ /mol	Molality	Activity	Log		Log	
			Molality	Activity	Gamma	
OH-	3.324e-05	1.954e-05	-4.478	-4.709	-0.231	-
2.26						
H+	8.516e-09	6.310e-09	-8.070	-8.200	-0.130	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.37						
C(4)	1.581e-03					
HCO3-	7.193e-04	4.730e-04	-3.143	-3.325	-0.182	
27.98						
NaCO3-	2.562e-04	1.867e-04	-3.591	-3.729	-0.137	
4.62						
CaCO3	1.862e-04	2.173e-04	-3.730	-3.663	0.067	-
14.50						
MgHCO3+	1.414e-04	8.607e-05	-3.850	-4.065	-0.215	
6.37						
MgCO3	9.429e-05	1.101e-04	-4.026	-3.958	0.067	-
17.09						
CaHCO3+	9.148e-05	6.174e-05	-4.039	-4.209	-0.171	
10.89						
NaHCO3	5.739e-05	6.700e-05	-4.241	-4.174	0.067	
1.80						
CO3-2	2.945e-05	5.504e-06	-4.531	-5.259	-0.728	-
3.37						
CO2	5.172e-06	6.038e-06	-5.286	-5.219	0.067	
36.47						
(CO2)2	1.641e-12	1.916e-12	-11.785	-11.718	0.067	
72.95						
Ca	3.500e-02					
Ca+2	3.371e-02	7.525e-03	-1.472	-2.123	-0.651	-
16.47						
CaSO4	1.012e-03	1.182e-03	-2.995	-2.927	0.067	
8.45						
CaCO3	1.862e-04	2.173e-04	-3.730	-3.663	0.067	-
14.50						
CaHCO3+	9.148e-05	6.174e-05	-4.039	-4.209	-0.171	
10.89						
CaOH+	2.665e-07	1.942e-07	-6.574	-6.712	-0.137	
(0)						
CaHSO4+	1.391e-10	1.014e-10	-9.857	-9.994	-0.137	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.486e-01	-0.243	-0.458	-0.215	
18.91						
H(0)	3.398e-28					
H2	1.699e-28	1.984e-28	-27.770	-27.703	0.067	
28.58						
Mg	4.800e-02					
Mg+2	4.371e-02	1.134e-02	-1.359	-1.945	-0.586	-
21.54						
MgSO4	3.829e-03	4.470e-03	-2.417	-2.350	0.067	
6.80						

MgOH+	2.248e-04	1.547e-04	-3.648	-3.811	-0.162	
(0)						
MgHCO3+	1.414e-04	8.607e-05	-3.850	-4.065	-0.215	
6.37						
MgCO3	9.429e-05	1.101e-04	-4.026	-3.958	0.067	-
17.09						
Na	4.450e-01					
Na+	4.427e-01	3.076e-01	-0.354	-0.512	-0.158	
0.64						
NaSO4-	1.988e-03	1.307e-03	-2.702	-2.884	-0.182	
19.44						
NaCO3-	2.562e-04	1.867e-04	-3.591	-3.729	-0.137	
4.62						
NaHCO3	5.739e-05	6.700e-05	-4.241	-4.174	0.067	
1.80						
NaOH	5.149e-16	6.012e-16	-15.288	-15.221	0.067	
(0)						
O(0)	4.210e-26					
O2	2.105e-26	2.458e-26	-25.677	-25.609	0.067	
32.59						
S(6)	1.100e-02					
SO4-2	4.171e-03	6.779e-04	-2.380	-3.169	-0.789	
20.21						
MgSO4	3.829e-03	4.470e-03	-2.417	-2.350	0.067	
6.80						
NaSO4-	1.988e-03	1.307e-03	-2.702	-2.884	-0.182	
19.44						
CaSO4	1.012e-03	1.182e-03	-2.995	-2.927	0.067	
8.45						
HSO4-	1.537e-09	1.121e-09	-8.813	-8.951	-0.137	
42.37						
CaHSO4+	1.391e-10	1.014e-10	-9.857	-9.994	-0.137	
(0)						

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

Phase	SI**	log IAP	log K(338 K,	1 atm)
Anhydrite	-0.52	-5.29	-4.77	CaSO4
Aragonite	1.31	-7.38	-8.69	CaCO3
Calcite	1.43	-7.38	-8.81	CaCO3
CO2(g)	-3.40	-5.22	-1.82	CO2
Dolomite	3.32	-14.59	-17.91	CaMg(CO3)2
Gypsum	-0.64	-5.31	-4.67	CaSO4:2H2O
H2(g)	-24.56	-27.70	-3.14	H2
H2O(g)	-0.62	-0.01	0.61	H2O
Halite	-2.57	-0.97	1.60	NaCl
O2(g)	-22.53	-25.61	-3.08	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.41 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 1atm, T variable\T=70.pqi

Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 1atm, T variable\T=70.pqi

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 70
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH = 8.200
 pe = 4.000
 Specific Conductance ($\mu\text{S}/\text{cm}$, 70°C) = 102419
 Density (g/cm^3) = 1.00168
 Volume (L) = 1.03249
 Activity of water = 0.981
 Ionic strength (mol/kgw) = $6.717\text{e-}01$
 Mass of water (kg) = $1.000\text{e+}00$
 Total carbon (mol/kg) = $1.470\text{e-}03$
 Total CO2 (mol/kg) = $1.470\text{e-}03$
 Temperature ($^\circ\text{C}$) = 70.00
 Electrical balance (eq) = $1.460\text{e-}02$
 Percent error, $100 \cdot (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = 1.24
 Iterations = 8
 Total H = $1.110137\text{e+}02$
 Total O = $5.555498\text{e+}01$

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

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	$4.295\text{e-}05$	$2.513\text{e-}05$	-4.367	-4.600	-0.233	-
2.36						
H+	$8.539\text{e-}09$	$6.310\text{e-}09$	-8.069	-8.200	-0.131	
0.00						
H2O	$5.551\text{e+}01$	$9.812\text{e-}01$	1.744	-0.008	0.000	
18.43						
C(4)	$1.470\text{e-}03$					
HCO3-	$6.292\text{e-}04$	$4.121\text{e-}04$	-3.201	-3.385	-0.184	
27.95						
NaCO3-	$2.743\text{e-}04$	$1.992\text{e-}04$	-3.562	-3.701	-0.139	
4.55						
CaCO3	$1.900\text{e-}04$	$2.218\text{e-}04$	-3.721	-3.654	0.067	-
14.49						
MgHCO3+	$1.281\text{e-}04$	$7.763\text{e-}05$	-3.892	-4.110	-0.218	
6.38						
MgCO3	$8.813\text{e-}05$	$1.029\text{e-}04$	-4.055	-3.988	0.067	-
17.09						
CaHCO3+	$8.071\text{e-}05$	$5.427\text{e-}05$	-4.093	-4.265	-0.172	
10.94						

NaHCO3	4.871e-05	5.686e-05	-4.312	-4.245	0.067	
1.80						
CO3-2	2.644e-05	4.863e-06	-4.578	-5.313	-0.735	-
3.99						
CO2	4.619e-06	5.391e-06	-5.335	-5.268	0.067	
36.77						
(CO2)2	1.444e-12	1.686e-12	-11.840	-11.773	0.067	
73.54						
Ca	3.500e-02					
Ca+2	3.374e-02	7.407e-03	-1.472	-2.130	-0.659	-
16.52						
CaSO4	9.863e-04	1.151e-03	-3.006	-2.939	0.067	
8.53						
CaCO3	1.900e-04	2.218e-04	-3.721	-3.654	0.067	-
14.49						
CaHCO3+	8.071e-05	5.427e-05	-4.093	-4.265	-0.172	
10.94						
CaOH+	2.632e-07	1.912e-07	-6.580	-6.719	-0.139	
(0)						
CaHSO4+	1.516e-10	1.101e-10	-9.819	-9.958	-0.139	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.469e-01	-0.243	-0.460	-0.217	
18.80						
H(0)	3.272e-28					
H2	1.636e-28	1.910e-28	-27.786	-27.719	0.067	
28.58						
Mg	4.800e-02					
Mg+2	4.349e-02	1.111e-02	-1.362	-1.954	-0.593	-
21.70						
MgSO4	3.980e-03	4.646e-03	-2.400	-2.333	0.067	
6.87						
MgOH+	3.123e-04	2.141e-04	-3.505	-3.669	-0.164	
(0)						
MgHCO3+	1.281e-04	7.763e-05	-3.892	-4.110	-0.218	
6.38						
MgCO3	8.813e-05	1.029e-04	-4.055	-3.988	0.067	-
17.09						
Na	4.450e-01					
Na+	4.427e-01	3.061e-01	-0.354	-0.514	-0.160	
0.72						
NaSO4-	1.957e-03	1.281e-03	-2.708	-2.892	-0.184	
19.01						
NaCO3-	2.743e-04	1.992e-04	-3.562	-3.701	-0.139	
4.55						
NaHCO3	4.871e-05	5.686e-05	-4.312	-4.245	0.067	
1.80						
NaOH	6.590e-16	7.692e-16	-15.181	-15.114	0.067	
(0)						
O(0)	7.829e-25					
O2	3.914e-25	4.569e-25	-24.407	-24.340	0.067	
32.79						
S(6)	1.100e-02					
SO4-2	4.077e-03	6.518e-04	-2.390	-3.186	-0.796	
20.21						
MgSO4	3.980e-03	4.646e-03	-2.400	-2.333	0.067	
6.87						

NaSO4-	1.957e-03	1.281e-03	-2.708	-2.892	-0.184
19.01					
CaSO4	9.863e-04	1.151e-03	-3.006	-2.939	0.067
8.53					
HSO4-	1.702e-09	1.236e-09	-8.769	-8.908	-0.139
42.41					
CaHSO4+	1.516e-10	1.101e-10	-9.819	-9.958	-0.139
(0)					

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

Phase	SI**	log IAP	log K(343 K,	1 atm)
Anhydrite	-0.48	-5.32	-4.84	CaSO4
Aragonite	1.31	-7.44	-8.75	CaCO3
Calcite	1.42	-7.44	-8.87	CaCO3
CO2(g)	-3.42	-5.27	-1.85	CO2
Dolomite	3.29	-14.71	-18.00	CaMg(CO3)2
Gypsum	-0.64	-5.33	-4.69	CaSO4:2H2O
H2(g)	-24.58	-27.72	-3.14	H2
H2O(g)	-0.52	-0.01	0.51	H2O
Halite	-2.58	-0.97	1.60	NaCl
O2(g)	-21.25	-24.34	-3.09	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.114 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 1atm, T variable\T=80.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 1atm, T variable\T=80.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 80
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kgw

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 80°C)	=	114163
Density (g/cm^3)	=	0.99572
Volume (L)	=	1.03866
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.706e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.198e-03
Total CO2 (mol/kg)	=	1.198e-03
Temperature (°C)	=	80.00
Electrical balance (eq)	=	1.460e-02

Percent error, $100 * (Cat - |An|) / (Cat + |An|) = 1.24$
Iterations = 9
Total H = 1.110137e+02
Total O = 5.555446e+01

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

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	6.927e-05	4.009e-05	-4.159	-4.397	-0.238	-
2.66						
H+	8.588e-09	6.310e-09	-8.066	-8.200	-0.134	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.54						
C(4)	1.198e-03					
HCO3-	4.509e-04	2.928e-04	-3.346	-3.533	-0.187	
27.82						
NaCO3-	2.831e-04	2.041e-04	-3.548	-3.690	-0.142	
4.25						
CaCO3	1.797e-04	2.097e-04	-3.745	-3.678	0.067	-
14.47						
MgHCO3+	9.900e-05	5.940e-05	-4.004	-4.226	-0.222	
6.35						
MgCO3	7.023e-05	8.196e-05	-4.153	-4.086	0.067	-
17.08						
CaHCO3+	5.928e-05	3.956e-05	-4.227	-4.403	-0.176	
11.03						
NaHCO3	3.289e-05	3.838e-05	-4.483	-4.416	0.067	
1.80						
CO3-2	1.953e-05	3.476e-06	-4.709	-5.459	-0.750	-
5.50						
CO2	3.516e-06	4.103e-06	-5.454	-5.387	0.067	
37.40						
(CO2) 2	1.001e-12	1.168e-12	-12.000	-11.933	0.067	
74.80						
Ca	3.500e-02					
Ca+2	3.383e-02	7.168e-03	-1.471	-2.145	-0.674	-
16.65						
CaSO4	9.344e-04	1.090e-03	-3.029	-2.962	0.067	
8.66						
CaCO3	1.797e-04	2.097e-04	-3.745	-3.678	0.067	-
14.47						
CaHCO3+	5.928e-05	3.956e-05	-4.227	-4.403	-0.176	
11.03						
CaOH+	2.567e-07	1.850e-07	-6.591	-6.733	-0.142	
(0)						
CaHSO4+	1.815e-10	1.308e-10	-9.741	-9.883	-0.142	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.432e-01	-0.243	-0.464	-0.222	
18.51						
H(0)	3.042e-28					

H2	1.521e-28	1.775e-28	-27.818	-27.751	0.067	
28.57						
Mg	4.800e-02					
Mg+2	4.299e-02	1.062e-02	-1.367	-1.974	-0.607	-
22.04						
MgSO4	4.259e-03	4.970e-03	-2.371	-2.304	0.067	
7.00						
MgOH+	5.832e-04	3.970e-04	-3.234	-3.401	-0.167	
(0)						
MgHCO3+	9.900e-05	5.940e-05	-4.004	-4.226	-0.222	
6.35						
MgCO3	7.023e-05	8.196e-05	-4.153	-4.086	0.067	-
17.08						
Na	4.450e-01					
Na+	4.428e-01	3.031e-01	-0.354	-0.518	-0.165	
0.88						
NaSO4-	1.896e-03	1.231e-03	-2.722	-2.910	-0.187	
18.01						
NaCO3-	2.831e-04	2.041e-04	-3.548	-3.690	-0.142	
4.25						
NaHCO3	3.289e-05	3.838e-05	-4.483	-4.416	0.067	
1.80						
NaOH	1.041e-15	1.215e-15	-14.982	-14.915	0.067	
(0)						
O(0)	2.111e-22					
O2	1.056e-22	1.232e-22	-21.976	-21.909	0.067	
33.17						
S(6)	1.100e-02					
MgSO4	4.259e-03	4.970e-03	-2.371	-2.304	0.067	
7.00						
SO4-2	3.911e-03	6.039e-04	-2.408	-3.219	-0.811	
20.04						
NaSO4-	1.896e-03	1.231e-03	-2.722	-2.910	-0.187	
18.01						
CaSO4	9.344e-04	1.090e-03	-3.029	-2.962	0.067	
8.66						
HSO4-	2.106e-09	1.518e-09	-8.676	-8.819	-0.142	
42.42						
CaHSO4+	1.815e-10	1.308e-10	-9.741	-9.883	-0.142	
(0)						

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

Phase	SI**	log IAP	log K(353 K,	1 atm)
Anhydrite	-0.39	-5.36	-4.98	CaSO4
Aragonite	1.27	-7.60	-8.88	CaCO3
Calcite	1.39	-7.60	-8.99	CaCO3
CO2(g)	-3.49	-5.39	-1.90	CO2
Dolomite	3.13	-15.04	-18.17	CaMg(CO3)2
Gypsum	-0.64	-5.38	-4.74	CaSO4:2H2O
H2(g)	-24.62	-27.75	-3.13	H2
H2O(g)	-0.34	-0.01	0.33	H2O
Halite	-2.59	-0.98	1.61	NaCl
O2(g)	-18.80	-21.91	-3.11	O2

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.11 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 1atm, T variable\T=90.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 1atm, T variable\T=90.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 90
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

--

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

--

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 90°C)	=	125834
Density (g/cm^3)	=	0.98930
Volume (L)	=	1.04539
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.694e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	8.224e-04
Total CO2 (mol/kg)	=	8.224e-04
Temperature (°C)	=	90.00
Electrical balance (eq)	=	1.460e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.24
Iterations	=	8
Total H	=	1.110140e+02
Total O	=	5.555383e+01

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

--

mole V Species cm^3/mol	Molality	Activity	Log		Log	
			Molality	Activity	Gamma	
OH-	1.070e-04	6.123e-05	-3.971	-4.213	-0.243	-
3.06						
H+	8.642e-09	6.310e-09	-8.063	-8.200	-0.137	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.66						
C(4)	8.224e-04					
HCO3-	2.717e-04	1.749e-04	-3.566	-3.757	-0.191	
27.60						
NaCO3-	2.342e-04	1.674e-04	-3.630	-3.776	-0.146	
3.76						

CaCO3	1.363e-04	1.590e-04	-3.866	-3.799	0.067	-
14.45						
MgHCO3+	6.461e-05	3.835e-05	-4.190	-4.416	-0.227	
6.29						
MgCO3	4.550e-05	5.309e-05	-4.342	-4.275	0.067	-
17.08						
CaHCO3+	3.731e-05	2.469e-05	-4.428	-4.607	-0.179	
11.09						
NaHCO3	1.869e-05	2.181e-05	-4.728	-4.661	0.067	
1.80						
CO3-2	1.183e-05	2.031e-06	-4.927	-5.692	-0.765	-
7.36						
CO2	2.302e-06	2.686e-06	-5.638	-5.571	0.067	
38.10						
(CO2) 2	5.015e-13	5.850e-13	-12.300	-12.233	0.067	
76.21						
Ca	3.500e-02					
Ca+2	3.394e-02	6.926e-03	-1.469	-2.160	-0.690	-
16.84						
CaSO4	8.846e-04	1.032e-03	-3.053	-2.986	0.067	
8.76						
CaCO3	1.363e-04	1.590e-04	-3.866	-3.799	0.067	-
14.45						
CaHCO3+	3.731e-05	2.469e-05	-4.428	-4.607	-0.179	
11.09						
CaOH+	2.501e-07	1.788e-07	-6.602	-6.748	-0.146	
(0)						
CaHSO4+	2.198e-10	1.571e-10	-9.658	-9.804	-0.146	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.393e-01	-0.243	-0.469	-0.227	
18.12						
H(0)	2.840e-28					
H2	1.420e-28	1.657e-28	-27.848	-27.781	0.067	
28.57						
Mg	4.800e-02					
Mg+2	4.234e-02	1.009e-02	-1.373	-1.996	-0.623	-
22.42						
MgSO4	4.502e-03	5.252e-03	-2.347	-2.280	0.067	
7.11						
MgOH+	1.045e-03	7.057e-04	-2.981	-3.151	-0.170	
(0)						
MgHCO3+	6.461e-05	3.835e-05	-4.190	-4.416	-0.227	
6.29						
MgCO3	4.550e-05	5.309e-05	-4.342	-4.275	0.067	-
17.08						
Na	4.450e-01					
Na+	4.429e-01	2.999e-01	-0.354	-0.523	-0.169	
1.02						
NaSO4-	1.839e-03	1.184e-03	-2.735	-2.927	-0.191	
16.80						
NaCO3-	2.342e-04	1.674e-04	-3.630	-3.776	-0.146	
3.76						
NaHCO3	1.869e-05	2.181e-05	-4.728	-4.661	0.067	
1.80						
NaOH	1.574e-15	1.836e-15	-14.803	-14.736	0.067	
(0)						

O(0)	4.184e-20					
O2	2.092e-20	2.441e-20	-19.679	-19.612	0.067	
33.54						
S(6)	1.100e-02					
MgSO4	4.502e-03	5.252e-03	-2.347	-2.280	0.067	
7.11						
SO4-2	3.774e-03	5.615e-04	-2.423	-3.251	-0.827	
19.66						
NaSO4-	1.839e-03	1.184e-03	-2.735	-2.927	-0.191	
16.80						
CaSO4	8.846e-04	1.032e-03	-3.053	-2.986	0.067	
8.76						
HSO4-	2.639e-09	1.886e-09	-8.579	-8.724	-0.146	
42.34						
CaHSO4+	2.198e-10	1.571e-10	-9.658	-9.804	-0.146	
(0)						

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

Phase	SI**	log IAP	log K(363 K,	1 atm)
Anhydrite	-0.29	-5.41	-5.12	CaSO4
Aragonite	1.16	-7.85	-9.02	CaCO3
Calcite	1.27	-7.85	-9.12	CaCO3
CO2(g)	-3.63	-5.57	-1.94	CO2
Dolomite	2.79	-15.54	-18.33	CaMg(CO3)2
Gypsum	-0.64	-5.43	-4.79	CaSO4:2H2O
H2(g)	-24.66	-27.78	-3.12	H2
H2O(g)	-0.17	-0.01	0.16	H2O
Halite	-2.61	-0.99	1.61	NaCl
O2(g)	-16.50	-19.61	-3.11	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.128 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 1atm, T variable\T=100.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 1atm, T variable\T=100.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 100
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kgg

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH = 8.200
pe = 4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 100°C) = 137325
Density (g/cm^3) = 0.98245

Volume (L) = 1.05266
 Activity of water = 0.981
 Ionic strength (mol/kgw) = 6.680e-01
 Mass of water (kg) = 1.000e+00
 Total carbon (mol/kg) = 2.839e-04
 Total CO2 (mol/kg) = 2.839e-04
 Temperature (°C) = 100.00
 Electrical balance (eq) = 1.460e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.24
 Iterations = 8
 Total H = 1.110145e+02
 Total O = 5.555302e+01

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

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm ³ /mol						
OH-	1.590e-04	8.984e-05	-3.799	-4.047	-0.248	-
3.59						
H+	8.698e-09	6.310e-09	-8.061	-8.200	-0.139	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.80						
C(4)	2.839e-04					
NaCO3-	9.379e-05	6.646e-05	-4.028	-4.177	-0.150	
3.04						
HCO3-	8.284e-05	5.283e-05	-4.082	-4.277	-0.195	
27.27						
CaCO3	4.958e-05	5.783e-05	-4.305	-4.238	0.067	-
14.43						
MgHCO3+	2.135e-05	1.253e-05	-4.671	-4.902	-0.231	
6.19						
MgCO3	1.443e-05	1.683e-05	-4.841	-4.774	0.067	-
17.07						
CaHCO3+	1.222e-05	8.013e-06	-4.913	-5.096	-0.183	
11.12						
NaHCO3	5.383e-06	6.278e-06	-5.269	-5.202	0.067	
1.80						
CO3-2	3.541e-06	5.857e-07	-5.451	-6.232	-0.781	-
9.60						
CO2	7.779e-07	9.073e-07	-6.109	-6.042	0.067	
38.89						
(CO2)2	6.551e-14	7.640e-14	-13.184	-13.117	0.067	
77.78						
Ca	3.500e-02					
Ca+2	3.410e-02	6.684e-03	-1.467	-2.175	-0.708	-
17.07						
CaSO4	8.387e-04	9.782e-04	-3.076	-3.010	0.067	
8.86						
CaCO3	4.958e-05	5.783e-05	-4.305	-4.238	0.067	-
14.43						
CaHCO3+	1.222e-05	8.013e-06	-4.913	-5.096	-0.183	
11.12						

CaOH+	2.435e-07	1.725e-07	-6.614	-6.763	-0.150	
(0)						
CaHSO4+	2.692e-10	1.908e-10	-9.570	-9.719	-0.150	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.353e-01	-0.243	-0.475	-0.232	
17.63						
H(0)	2.661e-28					
H2	1.331e-28	1.552e-28	-27.876	-27.809	0.067	
28.57						
Mg	4.800e-02					
Mg+2	4.147e-02	9.516e-03	-1.382	-2.022	-0.639	-
22.83						
MgSO4	4.701e-03	5.482e-03	-2.328	-2.261	0.067	
7.20						
MgOH+	1.796e-03	1.203e-03	-2.746	-2.920	-0.174	
(0)						
MgHCO3+	2.135e-05	1.253e-05	-4.671	-4.902	-0.231	
6.19						
MgCO3	1.443e-05	1.683e-05	-4.841	-4.774	0.067	-
17.07						
Na	4.450e-01					
Na+	4.431e-01	2.966e-01	-0.353	-0.528	-0.174	
1.15						
NaSO4-	1.790e-03	1.141e-03	-2.747	-2.943	-0.195	
15.36						
NaCO3-	9.379e-05	6.646e-05	-4.028	-4.177	-0.150	
3.04						
NaHCO3	5.383e-06	6.278e-06	-5.269	-5.202	0.067	
1.80						
NaOH	2.285e-15	2.665e-15	-14.641	-14.574	0.067	
(0)						
O(0)	6.245e-18					
O2	3.122e-18	3.642e-18	-17.506	-17.439	0.067	
33.90						
S(6)	1.100e-02					
MgSO4	4.701e-03	5.482e-03	-2.328	-2.261	0.067	
7.20						
SO4-2	3.671e-03	5.250e-04	-2.435	-3.280	-0.845	
19.08						
NaSO4-	1.790e-03	1.141e-03	-2.747	-2.943	-0.195	
15.36						
CaSO4	8.387e-04	9.782e-04	-3.076	-3.010	0.067	
8.86						
HSO4-	3.350e-09	2.374e-09	-8.475	-8.625	-0.150	
42.18						
CaHSO4+	2.692e-10	1.908e-10	-9.570	-9.719	-0.150	
(0)						

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

Phase	SI**	log IAP	log K(373 K,	1 atm)
Anhydrite	-0.19	-5.45	-5.26	CaSO4
Aragonite	0.76	-8.41	-9.17	CaCO3
Calcite	0.86	-8.41	-9.27	CaCO3

CO2(g)	-4.06	-6.04	-1.98	CO2
Dolomite	1.82	-16.66	-18.48	CaMg(CO3)2
Gypsum	-0.62	-5.47	-4.85	CaSO4:2H2O
H2(g)	-24.71	-27.81	-3.10	H2
H2O(g)	-0.01	-0.01	0.00	H2O
Halite	-2.62	-1.00	1.62	NaCl
O2(g)	-14.32	-17.44	-3.11	O2

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.121 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=40.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=40.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1

```

Ca      35
Mg      48
Na     445
S(6)   11
Alkalinity 2.4 as HCO3-
Cl     572
water  1 # kg
REACTION PRESSURE 1
10.89

```

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

```

pH = 8.200
pe = 4.000
Specific Conductance (µS/cm, 40°C) = 67832
Density (g/cm³) = 1.01647
Volume (L) = 1.01750
Activity of water = 0.981
Ionic strength (mol/kgw) = 6.753e-01
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 1.989e-03
Total CO2 (mol/kg) = 1.989e-03
Temperature (°C) = 40.00
Electrical balance (eq) = 1.460e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
Iterations = 7
Total H = 1.110141e+02
Total O = 5.555622e+01

```

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

mole V Species cm ³ /mol	Molality	Activity	Log	Log	Log	-
			Molality	Activity	Gamma	
OH- 2.19	7.568e-06	4.553e-06	-5.121	-5.342	-0.221	-

H+	8.413e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(4)	1.989e-03					
HCO3-	1.160e-03	7.764e-04	-2.935	-3.110	-0.174	
27.66						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
CO3-2	3.684e-05	7.386e-06	-4.434	-5.132	-0.698	-
1.66						
CO2	8.476e-06	9.902e-06	-5.072	-5.004	0.068	
35.16						
(CO2)2	2.427e-12	2.835e-12	-11.615	-11.547	0.068	
70.32						
Ca	3.500e-02					
Ca+2	3.360e-02	8.086e-03	-1.474	-2.092	-0.619	-
16.46						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
CaOH+	2.817e-07	2.087e-07	-6.550	-6.681	-0.130	
(0)						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	4.185e-28					
H2	2.093e-28	2.445e-28	-27.679	-27.612	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.244e-02	-1.350	-1.905	-0.555	-
20.81						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
MgOH+	3.650e-05	2.551e-05	-4.438	-4.593	-0.156	
(0)						
Na	4.450e-01					

Na+	4.426e-01	3.142e-01	-0.354	-0.503	-0.149
0.05					
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174
20.90					
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130
4.11					
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068
1.80					
NaOH	1.225e-16	1.431e-16	-15.912	-15.844	0.068
(0)					
O(0)	4.672e-33				
O2	2.336e-33	2.729e-33	-32.632	-32.564	0.068
31.40					
S(6)	1.100e-02				
SO4-2	4.738e-03	8.290e-04	-2.324	-3.081	-0.757
19.21					
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068
6.30					
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174
20.90					
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068
7.96					
HSO4-	9.700e-10	7.187e-10	-9.013	-9.143	-0.130
41.78					
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.72	-5.17	-4.45	CaSO4
Aragonite	1.22	-7.22	-8.45	CaCO3
Calcite	1.36	-7.22	-8.58	CaCO3
CO2(g)	-3.38	-5.00	-1.63	CO2
Dolomite	3.16	-14.26	-17.42	CaMg(CO3)2
Gypsum	-0.59	-5.19	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-29.58	-32.56	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
C	1.989e-03	1.989e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

pH = 8.196 Charge balance
 pe = 8.787 Adjusted to redox
 equilibrium
 Specific Conductance (µS/cm, 40°C) = 67833
 Density (g/cm³) = 1.01689
 Volume (L) = 1.01708
 Activity of water = 0.981
 Ionic strength (mol/kgw) = 6.753e-01
 Mass of water (kg) = 1.000e+00
 Total alkalinity (eq/kg) = 2.400e-03
 Total CO2 (mol/kg) = 1.989e-03
 Temperature (°C) = 40.00
 Pressure (atm) = 10.89
 Electrical balance (eq) = 1.460e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
 Iterations = 9
 Total H = 1.110141e+02
 Total O = 5.555622e+01

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

--

mole V Species cm³/mol	Molality	Activity	Log	Log	Log	Gamma
			Molality	Activity		
OH-	7.562e-06	4.551e-06	-5.121	-5.342	-0.221	-
2.19 H+	8.482e-09	6.362e-09	-8.072	-8.196	-0.125	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.15 C(-4)	0.000e+00					
36.63 CH4	0.000e+00	0.000e+00	-118.519	-118.452	0.068	
C(4)	1.989e-03					
HCO3-	1.159e-03	7.757e-04	-2.936	-3.110	-0.174	
27.66 MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.19 CaHCO3+	1.381e-04	9.477e-05	-3.860	-4.023	-0.164	
10.46						

CaCO3	1.242e-04	1.451e-04	-3.906	-3.838	0.068	-
14.49						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.051	-0.130	
4.19						
NaHCO3	1.093e-04	1.277e-04	-3.961	-3.894	0.068	
1.80						
MgCO3	9.459e-05	1.105e-04	-4.024	-3.957	0.068	-
17.02						
CO3-2	3.688e-05	7.401e-06	-4.433	-5.131	-0.698	-
1.58						
CO2	8.455e-06	9.878e-06	-5.073	-5.005	0.068	
35.15						
(CO2) 2	2.415e-12	2.821e-12	-11.617	-11.550	0.068	
70.30						
Ca	3.500e-02					
Ca+2	3.360e-02	8.093e-03	-1.474	-2.092	-0.618	-
16.39						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.99						
CaHCO3+	1.381e-04	9.477e-05	-3.860	-4.023	-0.164	
10.46						
CaCO3	1.242e-04	1.451e-04	-3.906	-3.838	0.068	-
14.49						
CaOH+	2.797e-07	2.073e-07	-6.553	-6.683	-0.130	
(0)						
CaHSO4+	9.537e-11	7.067e-11	-10.021	-10.151	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.567e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	1.124e-37					
H2	5.618e-38	6.563e-38	-37.250	-37.183	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.245e-02	-1.350	-1.905	-0.555	-
20.73						
MgSO4	2.987e-03	3.490e-03	-2.525	-2.457	0.068	
6.33						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.19						
MgCO3	9.459e-05	1.105e-04	-4.024	-3.957	0.068	-
17.02						
MgOH+	3.619e-05	2.530e-05	-4.441	-4.597	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.143e-01	-0.354	-0.503	-0.149	
0.08						
NaSO4-	2.137e-03	1.430e-03	-2.670	-2.845	-0.174	
20.83						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.051	-0.130	
4.19						
NaHCO3	1.093e-04	1.277e-04	-3.961	-3.894	0.068	
1.80						
NaOH	1.223e-16	1.429e-16	-15.912	-15.845	0.068	
(0)						
O(0)	6.355e-14					

O2	3.177e-14	3.712e-14	-13.498	-13.430	0.068
31.38					
S(-2)	0.000e+00				
HS-	0.000e+00	0.000e+00	-115.363	-115.584	-0.221
21.90					
H2S	0.000e+00	0.000e+00	-117.078	-117.010	0.068
37.19					
S-2	0.000e+00	0.000e+00	-119.147	-119.877	-0.730
(0)					
S(6)	1.100e-02				
SO4-2	4.740e-03	8.300e-04	-2.324	-3.081	-0.757
19.16					
MgSO4	2.987e-03	3.490e-03	-2.525	-2.457	0.068
6.33					
NaSO4-	2.137e-03	1.430e-03	-2.670	-2.845	-0.174
20.83					
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068
7.99					
HSO4-	9.707e-10	7.193e-10	-9.013	-9.143	-0.130
41.75					
CaHSO4+	9.537e-11	7.067e-11	-10.021	-10.151	-0.130
(0)					

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

Phase	SI**	log IAP	log K(313 K, 11 atm)	
Anhydrite	-0.73	-5.17	-4.44	CaSO4
Aragonite	1.21	-7.22	-8.44	CaCO3
Calcite	1.35	-7.22	-8.57	CaCO3
CH4(g)	-115.53	-118.45	-2.92	CH4
CO2(g)	-3.37	-5.01	-1.63	CO2
Dolomite	3.15	-14.26	-17.40	CaMg(CO3)2
Gypsum	-0.60	-5.19	-4.59	CaSO4:2H2O
H2(g)	-34.05	-37.18	-3.13	H2
H2O(g)	-1.14	-0.01	1.14	H2O
H2S(g)	-115.82	-123.78	-7.97	H2S
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-10.44	-13.43	-2.99	O2
Sulfur	-87.59	-83.04	4.54	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

 Reading input data for simulation 2.

 End of Run after 0.444 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=42.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=42.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 42
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
10.89

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01

Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

--

	pH	=	8.200
	pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 42°C)		=	70069
Density (g/cm^3)		=	1.01565
Volume (L)		=	1.01832
Activity of water		=	0.981
Ionic strength (mol/kgw)		=	6.751e-01
Mass of water (kg)		=	1.000e+00
Total carbon (mol/kg)		=	1.963e-03
Total CO2 (mol/kg)		=	1.963e-03
Temperature (°C)		=	42.00
Electrical balance (eq)		=	1.460e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$		=	1.23
Iterations		=	7
Total H		=	1.110140e+02
Total O		=	5.555615e+01

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

--

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm^3/mol						
OH-	8.634e-06	5.186e-06	-5.064	-5.285	-0.221	-
2.17						
H+	8.420e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.17						
C(4)	1.963e-03					
HCO3-	1.127e-03	7.534e-04	-2.948	-3.123	-0.175	
27.71						
MgHCO3+	1.945e-04	1.208e-04	-3.711	-3.918	-0.207	
6.19						
CaHCO3+	1.355e-04	9.285e-05	-3.868	-4.032	-0.164	
10.49						
NaCO3-	1.306e-04	9.662e-05	-3.884	-4.015	-0.131	
4.21						
CaCO3	1.299e-04	1.517e-04	-3.886	-3.819	0.068	-
14.55						
NaHCO3	1.039e-04	1.214e-04	-3.983	-3.916	0.068	
1.80						
MgCO3	9.631e-05	1.125e-04	-4.016	-3.949	0.068	-
17.10						
CO3-2	3.684e-05	7.349e-06	-4.434	-5.134	-0.700	-
1.70						
CO2	8.154e-06	9.526e-06	-5.089	-5.021	0.068	
35.26						

(CO2)2	2.372e-12	2.771e-12	-11.625	-11.557	0.068	
70.52						
Ca	3.500e-02					
Ca+2	3.361e-02	8.043e-03	-1.474	-2.095	-0.621	-
16.44						
CaSO4	1.127e-03	1.316e-03	-2.948	-2.881	0.068	
8.01						
CaHCO3+	1.355e-04	9.285e-05	-3.868	-4.032	-0.164	
10.49						
CaCO3	1.299e-04	1.517e-04	-3.886	-3.819	0.068	-
14.55						
CaOH+	2.805e-07	2.076e-07	-6.552	-6.683	-0.131	
(0)						
CaHSO4+	9.702e-11	7.180e-11	-10.013	-10.144	-0.131	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.560e-01	-0.243	-0.449	-0.206	
19.09						
H(0)	4.111e-28					
H2	2.056e-28	2.401e-28	-27.687	-27.620	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.461e-02	1.236e-02	-1.351	-1.908	-0.557	-
20.86						
MgSO4	3.061e-03	3.576e-03	-2.514	-2.447	0.068	
6.35						
MgHCO3+	1.945e-04	1.208e-04	-3.711	-3.918	-0.207	
6.19						
MgCO3	9.631e-05	1.125e-04	-4.016	-3.949	0.068	-
17.10						
MgOH+	4.271e-05	2.981e-05	-4.369	-4.526	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.138e-01	-0.354	-0.503	-0.149	
0.11						
NaSO4-	2.125e-03	1.420e-03	-2.673	-2.848	-0.175	
20.82						
NaCO3-	1.306e-04	9.662e-05	-3.884	-4.015	-0.131	
4.21						
NaHCO3	1.039e-04	1.214e-04	-3.983	-3.916	0.068	
1.80						
NaOH	1.393e-16	1.627e-16	-15.856	-15.789	0.068	
(0)						
O(0)	1.847e-32					
O2	9.236e-33	1.079e-32	-32.035	-31.967	0.068	
31.51						
S(6)	1.100e-02					
SO4-2	4.687e-03	8.157e-04	-2.329	-3.088	-0.759	
19.36						
MgSO4	3.061e-03	3.576e-03	-2.514	-2.447	0.068	
6.35						
NaSO4-	2.125e-03	1.420e-03	-2.673	-2.848	-0.175	
20.82						
CaSO4	1.127e-03	1.316e-03	-2.948	-2.881	0.068	
8.01						
HSO4-	1.003e-09	7.425e-10	-8.999	-9.129	-0.131	
41.86						

CaHSO4+ 9.702e-11 7.180e-11 -10.013 -10.144 -0.131
(0)

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

--

Phase	SI**	log IAP	log K(315 K,	1 atm)
Anhydrite	-0.71	-5.18	-4.48	CaSO4
Aragonite	1.23	-7.23	-8.46	CaCO3
Calcite	1.37	-7.23	-8.60	CaCO3
CO2(g)	-3.38	-5.02	-1.64	CO2
Dolomite	3.19	-14.27	-17.46	CaMg(CO3)2
Gypsum	-0.60	-5.20	-4.60	CaSO4:2H2O
H2(g)	-24.49	-27.62	-3.13	H2
H2O(g)	-1.10	-0.01	1.09	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-28.97	-31.97	-2.99	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.

Using pressure 1.

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

--

Elements	Molality	Moles
C	1.963e-03	1.963e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	8.196	Charge balance
	pe =	8.363	Adjusted to redox
equilibrium			
Specific Conductance (μS/cm, 42°C)	=	70067	
Density (g/cm³)	=	1.01606	
Volume (L)	=	1.01790	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.751e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	2.400e-03	
Total CO2 (mol/kg)	=	1.963e-03	

Temperature (°C) = 42.00
 Pressure (atm) = 10.89
 Electrical balance (eq) = 1.460e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
 Iterations = 10
 Total H = 1.110140e+02
 Total O = 5.555615e+01

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

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	8.628e-06	5.184e-06	-5.064	-5.285	-0.221	-
2.17						
H+	8.488e-09	6.361e-09	-8.071	-8.196	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-115.400	-115.332	0.068	
36.78						
C(4)	1.963e-03					
HCO3-	1.126e-03	7.527e-04	-2.948	-3.123	-0.175	
27.72						
MgHCO3+	1.945e-04	1.208e-04	-3.711	-3.918	-0.207	
6.22						
CaHCO3+	1.355e-04	9.288e-05	-3.868	-4.032	-0.164	
10.51						
NaCO3-	1.306e-04	9.664e-05	-3.884	-4.015	-0.131	
4.29						
CaCO3	1.301e-04	1.520e-04	-3.886	-3.818	0.068	-
14.48						
NaHCO3	1.049e-04	1.225e-04	-3.979	-3.912	0.068	
1.80						
MgCO3	9.640e-05	1.126e-04	-4.016	-3.948	0.068	-
17.02						
CO3-2	3.689e-05	7.364e-06	-4.433	-5.133	-0.700	-
1.62						
CO2	8.133e-06	9.501e-06	-5.090	-5.022	0.068	
35.25						
(CO2)2	2.360e-12	2.757e-12	-11.627	-11.560	0.068	
70.50						
Ca	3.500e-02					
Ca+2	3.361e-02	8.050e-03	-1.474	-2.094	-0.621	-
16.38						
CaSO4	1.127e-03	1.316e-03	-2.948	-2.881	0.068	
8.04						
CaHCO3+	1.355e-04	9.288e-05	-3.868	-4.032	-0.164	
10.51						
CaCO3	1.301e-04	1.520e-04	-3.886	-3.818	0.068	-
14.48						
CaOH+	2.786e-07	2.062e-07	-6.555	-6.686	-0.131	
(0)						

CaHSO4+	9.811e-11	7.261e-11	-10.008	-10.139	-0.131	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.561e-01	-0.243	-0.448	-0.206	
19.09						
H(0)	7.778e-37					
H2	3.889e-37	4.543e-37	-36.410	-36.343	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.461e-02	1.237e-02	-1.351	-1.908	-0.557	-
20.79						
MgSO4	3.058e-03	3.572e-03	-2.515	-2.447	0.068	
6.38						
MgHCO3+	1.945e-04	1.208e-04	-3.711	-3.918	-0.207	
6.22						
MgCO3	9.640e-05	1.126e-04	-4.016	-3.948	0.068	-
17.02						
MgOH+	4.235e-05	2.957e-05	-4.373	-4.529	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.138e-01	-0.354	-0.503	-0.149	
0.14						
NaSO4-	2.127e-03	1.422e-03	-2.672	-2.847	-0.175	
20.75						
NaCO3-	1.306e-04	9.664e-05	-3.884	-4.015	-0.131	
4.29						
NaHCO3	1.049e-04	1.225e-04	-3.979	-3.912	0.068	
1.80						
NaOH	1.392e-16	1.626e-16	-15.857	-15.789	0.068	
(0)						
O(0)	5.059e-15					
O2	2.529e-15	2.955e-15	-14.597	-14.529	0.068	
31.49						
S(-2)	0.000e+00					
HS-	0.000e+00	0.000e+00	-112.244	-112.465	-0.221	
21.95						
H2S	0.000e+00	0.000e+00	-113.978	-113.910	0.068	
37.20						
S-2	0.000e+00	0.000e+00	-115.973	-116.705	-0.732	
(0)						
S(6)	1.100e-02					
SO4-2	4.689e-03	8.166e-04	-2.329	-3.088	-0.759	
19.32						
MgSO4	3.058e-03	3.572e-03	-2.515	-2.447	0.068	
6.38						
NaSO4-	2.127e-03	1.422e-03	-2.672	-2.847	-0.175	
20.75						
CaSO4	1.127e-03	1.316e-03	-2.948	-2.881	0.068	
8.04						
HSO4-	1.004e-09	7.430e-10	-8.998	-9.129	-0.131	
41.83						
CaHSO4+	9.811e-11	7.261e-11	-10.008	-10.139	-0.131	
(0)						

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

Phase	SI**	log IAP	log K(315 K, 11 atm)	
Anhydrite	-0.71	-5.18	-4.47	CaSO4
Aragonite	1.23	-7.23	-8.45	CaCO3
Calcite	1.36	-7.23	-8.59	CaCO3
CH4(g)	-112.40	-115.33	-2.93	CH4
CO2(g)	-3.37	-5.02	-1.65	CO2
Dolomite	3.18	-14.27	-17.45	CaMg(CO3)2
Gypsum	-0.60	-5.20	-4.59	CaSO4:2H2O
H2(g)	-33.21	-36.34	-3.13	H2
H2O(g)	-1.10	-0.01	1.09	H2O
H2S(g)	-112.70	-120.66	-7.96	H2S
Halite	-2.54	-0.95	1.58	NaCl
O2(g)	-11.53	-14.53	-3.00	O2
Sulfur	-85.29	-80.79	4.50	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.132 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=45.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=45.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 45
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
10.89

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 45°C)	=	73449
Density (g/cm^3)	=	1.01436
Volume (L)	=	1.01961
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.747e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.922e-03
Total CO2 (mol/kg)	=	1.922e-03
Temperature (°C)	=	45.00
Electrical balance (eq)	=	1.460e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23
Iterations	=	7
Total H	=	1.110140e+02
Total O	=	5.555604e+01

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

--

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.047e-05	6.273e-06	-4.980	-5.202	-0.222	-
2.14						
H+	8.431e-09	6.310e-09	-8.074	-8.200	-0.126	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.19						
C(4)	1.922e-03					
HCO3-	1.077e-03	7.181e-04	-2.968	-3.144	-0.176	
27.79						
MgHCO3+	1.883e-04	1.166e-04	-3.725	-3.933	-0.208	
6.23						
NaCO3-	1.472e-04	1.088e-04	-3.832	-3.964	-0.132	
4.34						
CaCO3	1.388e-04	1.621e-04	-3.858	-3.790	0.067	-
14.55						
CaHCO3+	1.310e-04	8.963e-05	-3.883	-4.048	-0.165	
10.56						
MgCO3	9.848e-05	1.150e-04	-4.007	-3.939	0.067	-
17.10						
NaHCO3	9.732e-05	1.137e-04	-4.012	-3.944	0.067	
1.80						
CO3-2	3.663e-05	7.250e-06	-4.436	-5.140	-0.704	-
1.80						
CO2	7.698e-06	8.992e-06	-5.114	-5.046	0.067	
35.41						
(CO2)2	2.289e-12	2.674e-12	-11.640	-11.573	0.067	
70.81						
Ca	3.500e-02					
Ca+2	3.362e-02	7.978e-03	-1.473	-2.098	-0.625	-
16.43						
CaSO4	1.113e-03	1.300e-03	-2.954	-2.886	0.067	
8.08						
CaCO3	1.388e-04	1.621e-04	-3.858	-3.790	0.067	-
14.55						
CaHCO3+	1.310e-04	8.963e-05	-3.883	-4.048	-0.165	
10.56						
CaOH+	2.788e-07	2.059e-07	-6.555	-6.686	-0.132	
(0)						
CaHSO4+	1.013e-10	7.486e-11	-9.994	-10.126	-0.132	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.551e-01	-0.243	-0.450	-0.207	
19.10						
H(0)	4.004e-28					
H2	2.002e-28	2.339e-28	-27.699	-27.631	0.067	
28.59						
Mg	4.800e-02					
Mg+2	4.449e-02	1.223e-02	-1.352	-1.913	-0.561	-
20.95						

MgSO4	3.166e-03	3.698e-03	-2.499	-2.432	0.067	
6.42						
MgHCO3+	1.883e-04	1.166e-04	-3.725	-3.933	-0.208	
6.23						
MgCO3	9.848e-05	1.150e-04	-4.007	-3.939	0.067	-
17.10						
MgOH+	5.383e-05	3.751e-05	-4.269	-4.426	-0.157	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.130e-01	-0.354	-0.504	-0.151	
0.19						
NaSO4-	2.109e-03	1.406e-03	-2.676	-2.852	-0.176	
20.69						
NaCO3-	1.472e-04	1.088e-04	-3.832	-3.964	-0.132	
4.34						
NaHCO3	9.732e-05	1.137e-04	-4.012	-3.944	0.067	
1.80						
NaOH	1.681e-16	1.964e-16	-15.774	-15.707	0.067	
(0)						
O(0)	1.406e-31					
O2	7.029e-32	8.210e-32	-31.153	-31.086	0.067	
31.67						
S(6)	1.100e-02					
SO4-2	4.612e-03	7.961e-04	-2.336	-3.099	-0.763	
19.56						
MgSO4	3.166e-03	3.698e-03	-2.499	-2.432	0.067	
6.42						
NaSO4-	2.109e-03	1.406e-03	-2.676	-2.852	-0.176	
20.69						
CaSO4	1.113e-03	1.300e-03	-2.954	-2.886	0.067	
8.08						
HSO4-	1.056e-09	7.804e-10	-8.976	-9.108	-0.132	
41.96						
CaHSO4+	1.013e-10	7.486e-11	-9.994	-10.126	-0.132	
(0)						

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

Phase	SI**	log IAP	log K(318 K,	1 atm)
Anhydrite	-0.68	-5.20	-4.51	CaSO4
Aragonite	1.25	-7.24	-8.49	CaCO3
Calcite	1.38	-7.24	-8.62	CaCO3
CO2(g)	-3.38	-5.05	-1.67	CO2
Dolomite	3.23	-14.29	-17.52	CaMg(CO3)2
Gypsum	-0.61	-5.21	-4.61	CaSO4:2H2O
H2(g)	-24.50	-27.63	-3.13	H2
H2O(g)	-1.03	-0.01	1.03	H2O
Halite	-2.54	-0.95	1.59	NaCl
O2(g)	-28.08	-31.09	-3.01	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.

Using pressure 1.

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

Elements	Molality	Moles
C	1.922e-03	1.922e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

	pH =	8.197	Charge balance
	pe =	8.208	Adjusted to redox
equilibrium			
	Specific Conductance ($\mu\text{S}/\text{cm}$, 45°C)	=	73444
	Density (g/cm^3)	=	1.01478
	Volume (L)	=	1.01919
	Activity of water	=	0.981
	Ionic strength (mol/kgw)	=	6.747e-01
	Mass of water (kg)	=	1.000e+00
	Total alkalinity (eq/kg)	=	2.400e-03
	Total CO2 (mol/kg)	=	1.922e-03
	Temperature (°C)	=	45.00
	Pressure (atm)	=	10.89
	Electrical balance (eq)	=	1.460e-02
	Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23
	Iterations	=	10
	Total H	=	1.110140e+02
	Total O	=	5.555604e+01

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

mole V Species cm^3/mol	Molality	Activity	Log		Log	
			Molality	Activity	Gamma	
OH-	1.047e-05	6.272e-06	-4.980	-5.203	-0.222	-
2.15						
H+	8.497e-09	6.360e-09	-8.071	-8.197	-0.126	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.19						
C(-4)	0.000e+00					

CH4	0.000e+00	0.000e+00	-114.566	-114.499	0.067	
36.99						
C (4)	1.922e-03					
HCO3-	1.075e-03	7.174e-04	-2.968	-3.144	-0.176	
27.80						
MgHCO3+	1.882e-04	1.166e-04	-3.725	-3.933	-0.208	
6.26						
NaCO3-	1.472e-04	1.088e-04	-3.832	-3.963	-0.131	
4.42						
CaCO3	1.390e-04	1.624e-04	-3.857	-3.789	0.067	-
14.48						
CaHCO3+	1.310e-04	8.965e-05	-3.883	-4.047	-0.165	
10.58						
MgCO3	9.858e-05	1.152e-04	-4.006	-3.939	0.067	-
17.02						
NaHCO3	9.821e-05	1.147e-04	-4.008	-3.940	0.067	
1.80						
CO3-2	3.669e-05	7.267e-06	-4.436	-5.139	-0.703	-
1.72						
CO2	7.676e-06	8.966e-06	-5.115	-5.047	0.067	
35.40						
(CO2) 2	2.276e-12	2.659e-12	-11.643	-11.575	0.067	
70.80						
Ca	3.500e-02					
Ca+2	3.362e-02	7.985e-03	-1.473	-2.098	-0.624	-
16.36						
CaSO4	1.113e-03	1.300e-03	-2.953	-2.886	0.067	
8.11						
CaCO3	1.390e-04	1.624e-04	-3.857	-3.789	0.067	-
14.48						
CaHCO3+	1.310e-04	8.965e-05	-3.883	-4.047	-0.165	
10.58						
CaOH+	2.769e-07	2.046e-07	-6.558	-6.689	-0.131	
(0)						
CaHSO4+	1.025e-10	7.569e-11	-9.989	-10.121	-0.131	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.552e-01	-0.243	-0.450	-0.207	
19.10						
H (0)	1.546e-36					
H2	7.728e-37	9.027e-37	-36.112	-36.044	0.067	
28.59						
Mg	4.800e-02					
Mg+2	4.450e-02	1.224e-02	-1.352	-1.912	-0.561	-
20.87						
MgSO4	3.163e-03	3.695e-03	-2.500	-2.432	0.067	
6.45						
MgHCO3+	1.882e-04	1.166e-04	-3.725	-3.933	-0.208	
6.26						
MgCO3	9.858e-05	1.152e-04	-4.006	-3.939	0.067	-
17.02						
MgOH+	5.339e-05	3.721e-05	-4.273	-4.429	-0.157	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.131e-01	-0.354	-0.504	-0.150	
0.22						

NaSO4-	2.110e-03	1.408e-03	-2.676	-2.851	-0.176
20.63					
NaCO3-	1.472e-04	1.088e-04	-3.832	-3.963	-0.131
4.42					
NaHCO3	9.821e-05	1.147e-04	-4.008	-3.940	0.067
1.80					
NaOH	1.680e-16	1.962e-16	-15.775	-15.707	0.067
(0)					
O(0)	9.250e-15				
O2	4.625e-15	5.402e-15	-14.335	-14.267	0.067
31.65					
S(-2)	0.000e+00				
HS-	0.000e+00	0.000e+00	-111.408	-111.631	-0.222
22.00					
H2S	0.000e+00	0.000e+00	-113.170	-113.102	0.067
37.21					
S-2	0.000e+00	0.000e+00	-115.055	-115.791	-0.736
(0)					
S(6)	1.100e-02				
SO4-2	4.613e-03	7.970e-04	-2.336	-3.099	-0.763
19.52					
MgSO4	3.163e-03	3.695e-03	-2.500	-2.432	0.067
6.45					
NaSO4-	2.110e-03	1.408e-03	-2.676	-2.851	-0.176
20.63					
CaSO4	1.113e-03	1.300e-03	-2.953	-2.886	0.067
8.11					
HSO4-	1.057e-09	7.808e-10	-8.976	-9.107	-0.131
41.93					
CaHSO4+	1.025e-10	7.569e-11	-9.989	-10.121	-0.131
(0)					

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

Phase	SI**	log IAP	log K(318 K, 11 atm)	
Anhydrite	-0.69	-5.20	-4.51	CaSO4
Aragonite	1.24	-7.24	-8.48	CaCO3
Calcite	1.37	-7.24	-8.61	CaCO3
CH4(g)	-111.55	-114.50	-2.94	CH4
CO2(g)	-3.37	-5.05	-1.68	CO2
Dolomite	3.22	-14.29	-17.51	CaMg(CO3)2
Gypsum	-0.61	-5.21	-4.60	CaSO4:2H2O
H2(g)	-32.91	-36.04	-3.14	H2
H2O(g)	-1.03	-0.01	1.02	H2O
H2S(g)	-111.87	-119.83	-7.96	H2S
Halite	-2.54	-0.95	1.59	NaCl
O2(g)	-11.25	-14.27	-3.01	O2
Sulfur	-84.73	-80.29	4.44	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.136 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=49.pqi

Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=49.pqi

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 49
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
10.89

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 49°C)	=	77999
Density (g/cm^3)	=	1.01257
Volume (L)	=	1.02142
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.742e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.864e-03
Total CO2 (mol/kg)	=	1.864e-03
Temperature (°C)	=	49.00
Electrical balance (eq)	=	1.460e-02
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23
Iterations	=	7
Total H	=	1.110139e+02
Total O	=	5.555589e+01

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

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	1.343e-05	8.018e-06	-4.872	-5.096	-0.224	-
2.12 H+	8.447e-09	6.310e-09	-8.073	-8.200	-0.127	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.23 C(4)	1.864e-03					
HCO3-	1.007e-03	6.700e-04	-2.997	-3.174	-0.177	
27.86 MgHCO3+	1.796e-04	1.109e-04	-3.746	-3.955	-0.209	
6.28 NaCO3-	1.702e-04	1.254e-04	-3.769	-3.902	-0.133	
4.47 CaCO3	1.504e-04	1.757e-04	-3.823	-3.755	0.067	-
14.54						

CaHCO3+	1.242e-04	8.475e-05	-3.906	-4.072	-0.166	
10.64						
MgCO3	1.003e-04	1.171e-04	-3.999	-3.931	0.067	-
17.10						
NaHCO3	8.875e-05	1.037e-04	-4.052	-3.984	0.067	
1.80						
CO3-2	3.597e-05	7.042e-06	-4.444	-5.152	-0.708	-
1.99						
CO2	7.130e-06	8.327e-06	-5.147	-5.080	0.067	
35.61						
(CO2) 2	2.174e-12	2.540e-12	-11.663	-11.595	0.067	
71.22						
Ca	3.500e-02					
Ca+2	3.363e-02	7.891e-03	-1.473	-2.103	-0.630	-
16.42						
CaSO4	1.094e-03	1.278e-03	-2.961	-2.894	0.067	
8.17						
CaCO3	1.504e-04	1.757e-04	-3.823	-3.755	0.067	-
14.54						
CaHCO3+	1.242e-04	8.475e-05	-3.906	-4.072	-0.166	
10.64						
CaOH+	2.764e-07	2.036e-07	-6.558	-6.691	-0.133	
(0)						
CaHSO4+	1.076e-10	7.927e-11	-9.968	-10.101	-0.133	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.539e-01	-0.243	-0.451	-0.209	
19.10						
H(0)	3.869e-28					
H2	1.934e-28	2.259e-28	-27.713	-27.646	0.067	
28.59						
Mg	4.800e-02					
Mg+2	4.434e-02	1.206e-02	-1.353	-1.919	-0.566	-
21.06						
MgSO4	3.305e-03	3.860e-03	-2.481	-2.413	0.067	
6.51						
MgHCO3+	1.796e-04	1.109e-04	-3.746	-3.955	-0.209	
6.28						
MgCO3	1.003e-04	1.171e-04	-3.999	-3.931	0.067	-
17.10						
MgOH+	7.277e-05	5.059e-05	-4.138	-4.296	-0.158	
(0)						
Na	4.450e-01					
Na+	4.427e-01	3.120e-01	-0.354	-0.506	-0.152	
0.30						
NaSO4-	2.086e-03	1.387e-03	-2.681	-2.858	-0.177	
20.50						
NaCO3-	1.702e-04	1.254e-04	-3.769	-3.902	-0.133	
4.47						
NaHCO3	8.875e-05	1.037e-04	-4.052	-3.984	0.067	
1.80						
NaOH	2.142e-16	2.501e-16	-15.669	-15.602	0.067	
(0)						
O(0)	1.984e-30					
O2	9.921e-31	1.159e-30	-30.003	-29.936	0.067	
31.88						
S(6)	1.100e-02					

SO4-2	4.516e-03	7.707e-04	-2.345	-3.113	-0.768
19.78					
MgSO4	3.305e-03	3.860e-03	-2.481	-2.413	0.067
6.51					
NaSO4-	2.086e-03	1.387e-03	-2.681	-2.858	-0.177
20.50					
CaSO4	1.094e-03	1.278e-03	-2.961	-2.894	0.067
8.17					
HSO4-	1.134e-09	8.355e-10	-8.945	-9.078	-0.133
42.08					
CaHSO4+	1.076e-10	7.927e-11	-9.968	-10.101	-0.133
(0)					

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

--

Phase	SI**	log IAP	log K(322 K,	1 atm)
Anhydrite	-0.65	-5.22	-4.56	CaSO4
Aragonite	1.27	-7.26	-8.53	CaCO3
Calcite	1.40	-7.26	-8.65	CaCO3
CO2(g)	-3.38	-5.08	-1.70	CO2
Dolomite	3.28	-14.33	-17.61	CaMg(CO3)2
Gypsum	-0.62	-5.23	-4.62	CaSO4:2H2O
H2(g)	-24.51	-27.65	-3.14	H2
H2O(g)	-0.95	-0.01	0.94	H2O
Halite	-2.54	-0.96	1.59	NaCl
O2(g)	-26.91	-29.94	-3.03	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.

Using pressure 1.

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

--

Elements	Molality	Moles
C	1.864e-03	1.864e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

pH = 8.197 Charge balance

```

pe = 7.897 Adjusted to redox
equilibrium
  Specific Conductance (µS/cm, 49°C) = 77988
    Density (g/cm³) = 1.01298
      Volume (L) = 1.02100
        Activity of water = 0.981
          Ionic strength (mol/kgw) = 6.742e-01
            Mass of water (kg) = 1.000e+00
              Total alkalinity (eq/kg) = 2.400e-03
                Total CO2 (mol/kg) = 1.864e-03
                  Temperature (°C) = 49.00
                    Pressure (atm) = 10.89
                      Electrical balance (eq) = 1.460e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
  Iterations = 10
    Total H = 1.110139e+02
    Total O = 5.555589e+01

```

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

mole V Species cm³/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	1.343e-05	8.018e-06	-4.872	-5.096	-0.224	-
2.13 H+	8.510e-09	6.357e-09	-8.070	-8.197	-0.127	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.22 C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-112.617	-112.550	0.067	
37.27 C(4)	1.864e-03					
HCO3-	1.006e-03	6.693e-04	-2.997	-3.174	-0.177	
27.87 MgHCO3+	1.796e-04	1.109e-04	-3.746	-3.955	-0.209	
6.31 NaCO3-	1.703e-04	1.255e-04	-3.769	-3.901	-0.133	
4.56 CaCO3	1.507e-04	1.760e-04	-3.822	-3.754	0.067	-
14.47 CaHCO3+	1.242e-04	8.476e-05	-3.906	-4.072	-0.166	
10.66 MgCO3	1.004e-04	1.173e-04	-3.998	-3.931	0.067	-
17.02 NaHCO3	8.955e-05	1.046e-04	-4.048	-3.980	0.067	
1.80 CO3-2	3.603e-05	7.060e-06	-4.443	-5.151	-0.708	-
1.91 CO2	7.106e-06	8.300e-06	-5.148	-5.081	0.067	
35.60 (CO2)2	2.160e-12	2.523e-12	-11.665	-11.598	0.067	
71.20 Ca	3.500e-02					

Ca ²⁺	3.363e-02	7.898e-03	-1.473	-2.103	-0.629	-
16.35						
CaSO ₄	1.094e-03	1.278e-03	-2.961	-2.894	0.067	
8.19						
CaCO ₃	1.507e-04	1.760e-04	-3.822	-3.754	0.067	-
14.47						
CaHCO ₃ ⁺	1.242e-04	8.476e-05	-3.906	-4.072	-0.166	
10.66						
CaOH ⁺	2.747e-07	2.024e-07	-6.561	-6.694	-0.133	
(0)						
CaHSO ₄ ⁺	1.087e-10	8.012e-11	-9.964	-10.096	-0.133	
(0)						
Cl	5.720e-01					
Cl ⁻	5.720e-01	3.540e-01	-0.243	-0.451	-0.208	
19.10						
H(0)	6.234e-36					
H ₂	3.117e-36	3.641e-36	-35.506	-35.439	0.067	
28.58						
Mg	4.800e-02					
Mg ²⁺	4.435e-02	1.207e-02	-1.353	-1.918	-0.565	-
20.98						
MgSO ₄	3.302e-03	3.856e-03	-2.481	-2.414	0.067	
6.53						
MgHCO ₃ ⁺	1.796e-04	1.109e-04	-3.746	-3.955	-0.209	
6.31						
MgCO ₃	1.004e-04	1.173e-04	-3.998	-3.931	0.067	-
17.02						
MgOH ⁺	7.220e-05	5.021e-05	-4.141	-4.299	-0.158	
(0)						
Na	4.450e-01					
Na ⁺	4.427e-01	3.121e-01	-0.354	-0.506	-0.152	
0.33						
NaSO ₄ ⁻	2.088e-03	1.389e-03	-2.680	-2.857	-0.177	
20.44						
NaCO ₃ ⁻	1.703e-04	1.255e-04	-3.769	-3.901	-0.133	
4.56						
NaHCO ₃	8.955e-05	1.046e-04	-4.048	-3.980	0.067	
1.80						
NaOH	2.141e-16	2.500e-16	-15.669	-15.602	0.067	
(0)						
O(0)	7.492e-15					
O ₂	3.746e-15	4.375e-15	-14.426	-14.359	0.067	
31.85						
S(-2)	0.000e+00					
HS ⁻	0.000e+00	0.000e+00	-109.451	-109.675	-0.224	
22.06						
H ₂ S	0.000e+00	0.000e+00	-111.247	-111.179	0.067	
37.22						
S(-2)	0.000e+00	0.000e+00	-112.992	-113.732	-0.740	
(0)						
S(6)	1.100e-02					
SO ₄ ⁻²	4.517e-03	7.715e-04	-2.345	-3.113	-0.767	
19.75						
MgSO ₄	3.302e-03	3.856e-03	-2.481	-2.414	0.067	
6.53						
NaSO ₄ ⁻	2.088e-03	1.389e-03	-2.680	-2.857	-0.177	
20.44						

CaSO4	1.094e-03	1.278e-03	-2.961	-2.894	0.067
8.19					
HSO4-	1.134e-09	8.357e-10	-8.945	-9.078	-0.133
42.05					
CaHSO4+	1.087e-10	8.012e-11	-9.964	-10.096	-0.133
(0)					

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

Phase	SI**	log IAP	log K(322 K, 11 atm)	
Anhydrite	-0.66	-5.22	-4.56	CaSO4
Aragonite	1.26	-7.25	-8.52	CaCO3
Calcite	1.39	-7.25	-8.64	CaCO3
CH4(g)	-109.59	-112.55	-2.96	CH4
CO2(g)	-3.37	-5.08	-1.71	CO2
Dolomite	3.26	-14.32	-17.59	CaMg(CO3)2
Gypsum	-0.62	-5.23	-4.61	CaSO4:2H2O
H2(g)	-32.30	-35.44	-3.14	H2
H2O(g)	-0.94	-0.01	0.93	H2O
H2S(g)	-109.92	-117.87	-7.95	H2S
Halite	-2.55	-0.96	1.59	NaCl
O2(g)	-11.33	-14.36	-3.03	O2
Sulfur	-83.35	-78.99	4.36	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.128 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=50.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=50.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 50
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
10.89

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 50°C)	=	79144
Density (g/cm^3)	=	1.01210
Volume (L)	=	1.02188
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.741e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.849e-03

Total CO2 (mol/kg) = 1.849e-03
 Temperature (°C) = 50.00
 Electrical balance (eq) = 1.460e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
 Iterations = 7
 Total H = 1.110139e+02
 Total O = 5.555585e+01

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

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm ³ /mol						
OH-	1.427e-05	8.512e-06	-4.846	-5.070	-0.224	-
2.12						
H+	8.451e-09	6.310e-09	-8.073	-8.200	-0.127	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.23						
C(4)	1.849e-03					
HCO3-	9.895e-04	6.578e-04	-3.005	-3.182	-0.177	
27.88						
MgHCO3+	1.774e-04	1.094e-04	-3.751	-3.961	-0.210	
6.29						
NaCO3-	1.760e-04	1.296e-04	-3.754	-3.887	-0.133	
4.50						
CaCO3	1.533e-04	1.790e-04	-3.815	-3.747	0.067	-
14.53						
CaHCO3+	1.224e-04	8.344e-05	-3.912	-4.079	-0.166	
10.66						
MgCO3	1.005e-04	1.174e-04	-3.998	-3.930	0.067	-
17.10						
NaHCO3	8.664e-05	1.012e-04	-4.062	-3.995	0.067	
1.80						
CO3-2	3.573e-05	6.977e-06	-4.447	-5.156	-0.709	-
2.05						
CO2	6.994e-06	8.168e-06	-5.155	-5.088	0.067	
35.66						
(CO2)2	2.145e-12	2.505e-12	-11.669	-11.601	0.067	
71.32						
Ca	3.500e-02					
Ca+2	3.364e-02	7.869e-03	-1.473	-2.104	-0.631	-
16.41						
CaSO4	1.089e-03	1.272e-03	-2.963	-2.896	0.067	
8.19						
CaCO3	1.533e-04	1.790e-04	-3.815	-3.747	0.067	-
14.53						
CaHCO3+	1.224e-04	8.344e-05	-3.912	-4.079	-0.166	
10.66						
CaOH+	2.758e-07	2.031e-07	-6.559	-6.692	-0.133	
(0)						
CaHSO4+	1.092e-10	8.043e-11	-9.962	-10.095	-0.133	
(0)						
Cl	5.720e-01					

Cl-	5.720e-01	3.536e-01	-0.243	-0.452	-0.209	
19.10						
H(0)	3.836e-28					
H2	1.918e-28	2.240e-28	-27.717	-27.650	0.067	
28.59						
Mg	4.800e-02					
Mg+2	4.430e-02	1.201e-02	-1.354	-1.920	-0.567	-
21.09						
MgSO4	3.339e-03	3.900e-03	-2.476	-2.409	0.067	
6.53						
MgHCO3+	1.774e-04	1.094e-04	-3.751	-3.961	-0.210	
6.29						
MgCO3	1.005e-04	1.174e-04	-3.998	-3.930	0.067	-
17.10						
MgOH+	7.837e-05	5.445e-05	-4.106	-4.264	-0.158	
(0)						
Na	4.450e-01					
Na+	4.427e-01	3.117e-01	-0.354	-0.506	-0.152	
0.32						
NaSO4-	2.080e-03	1.382e-03	-2.682	-2.859	-0.177	
20.45						
NaCO3-	1.760e-04	1.296e-04	-3.754	-3.887	-0.133	
4.50						
NaHCO3	8.664e-05	1.012e-04	-4.062	-3.995	0.067	
1.80						
NaOH	2.272e-16	2.653e-16	-15.644	-15.576	0.067	
(0)						
O(0)	3.807e-30					
O2	1.903e-30	2.223e-30	-29.720	-29.653	0.067	
31.92						
S(6)	1.100e-02					
SO4-2	4.492e-03	7.645e-04	-2.348	-3.117	-0.769	
19.83						
MgSO4	3.339e-03	3.900e-03	-2.476	-2.409	0.067	
6.53						
NaSO4-	2.080e-03	1.382e-03	-2.682	-2.859	-0.177	
20.45						
CaSO4	1.089e-03	1.272e-03	-2.963	-2.896	0.067	
8.19						
HSO4-	1.155e-09	8.502e-10	-8.938	-9.070	-0.133	
42.11						
CaHSO4+	1.092e-10	8.043e-11	-9.962	-10.095	-0.133	
(0)						

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

Phase	SI**	log IAP	log K(323 K,	1 atm)
Anhydrite	-0.65	-5.22	-4.58	CaSO4
Aragonite	1.28	-7.26	-8.54	CaCO3
Calcite	1.40	-7.26	-8.66	CaCO3
CO2(g)	-3.38	-5.09	-1.71	CO2
Dolomite	3.29	-14.34	-17.63	CaMg(CO3)2
Gypsum	-0.62	-5.24	-4.62	CaSO4:2H2O
H2(g)	-24.51	-27.65	-3.14	H2
H2O(g)	-0.92	-0.01	0.92	H2O

Halite	-2.55	-0.96	1.59	NaCl
O2(g)	-26.62	-29.65	-3.03	O2

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
 Using pressure 1.

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

Elements	Molality	Moles
C	1.849e-03	1.849e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

	pH =	8.197	Charge balance
	pe =	-2.723	Adjusted to redox
equilibrium			
Specific Conductance ($\mu\text{S}/\text{cm}$, 50°C)	=	79131	
Density (g/cm^3)	=	1.01252	
Volume (L)	=	1.02146	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.741e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	2.400e-03	
Total CO2 (mol/kg)	=	1.849e-03	
Temperature (°C)	=	50.00	
Pressure (atm)	=	10.89	
Electrical balance (eq)	=	1.460e-02	
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23	
Iterations	=	15	
Total H	=	1.110139e+02	
Total O	=	5.555585e+01	

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

			Log	Log	Log	
mole V	Species	Molality	Activity	Molality	Activity	Gamma
cm^3/mol						

OH-	1.427e-05	8.514e-06	-4.846	-5.070	-0.224	-
2.14						
H+	8.513e-09	6.357e-09	-8.070	-8.197	-0.127	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.23						
C(-4)	1.630e-28					
CH4	1.630e-28	1.904e-28	-27.788	-27.720	0.067	
37.34						
C(4)	1.849e-03					
HCO3-	9.882e-04	6.571e-04	-3.005	-3.182	-0.177	
27.89						
MgHCO3+	1.774e-04	1.095e-04	-3.751	-3.961	-0.210	
6.32						
NaCO3-	1.761e-04	1.297e-04	-3.754	-3.887	-0.133	
4.58						
CaCO3	1.536e-04	1.794e-04	-3.814	-3.746	0.067	-
14.47						
CaHCO3+	1.224e-04	8.345e-05	-3.912	-4.079	-0.166	
10.68						
MgCO3	1.007e-04	1.176e-04	-3.997	-3.930	0.067	-
17.02						
NaHCO3	8.743e-05	1.021e-04	-4.058	-3.991	0.067	
1.80						
CO3-2	3.580e-05	6.996e-06	-4.446	-5.155	-0.709	-
1.97						
CO2	6.970e-06	8.141e-06	-5.157	-5.089	0.067	
35.65						
(CO2) 2	2.130e-12	2.488e-12	-11.672	-11.604	0.067	
71.30						
Ca	3.500e-02					
Ca+2	3.363e-02	7.875e-03	-1.473	-2.104	-0.631	-
16.35						
CaSO4	1.089e-03	1.272e-03	-2.963	-2.896	0.067	
8.21						
CaCO3	1.536e-04	1.794e-04	-3.814	-3.746	0.067	-
14.47						
CaHCO3+	1.224e-04	8.345e-05	-3.912	-4.079	-0.166	
10.68						
CaOH+	2.741e-07	2.019e-07	-6.562	-6.695	-0.133	
(0)						
CaHSO4+	1.104e-10	8.129e-11	-9.957	-10.090	-0.133	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.537e-01	-0.243	-0.451	-0.209	
19.10						
H(0)	1.075e-14					
H2	5.376e-15	6.279e-15	-14.270	-14.202	0.067	
28.58						
Mg	4.800e-02					
Mg+2	4.431e-02	1.202e-02	-1.354	-1.920	-0.566	-
21.01						
MgSO4	3.336e-03	3.896e-03	-2.477	-2.409	0.067	
6.56						
MgHCO3+	1.774e-04	1.095e-04	-3.751	-3.961	-0.210	
6.32						

MgCO3	1.007e-04	1.176e-04	-3.997	-3.930	0.067	-
17.02						
MgOH+	7.776e-05	5.404e-05	-4.109	-4.267	-0.158	
(0)						
Na	4.450e-01					
Na+	4.427e-01	3.118e-01	-0.354	-0.506	-0.152	
0.35						
NaSO4-	2.082e-03	1.384e-03	-2.682	-2.859	-0.177	
20.38						
NaCO3-	1.761e-04	1.297e-04	-3.754	-3.887	-0.133	
4.58						
NaHCO3	8.743e-05	1.021e-04	-4.058	-3.991	0.067	
1.80						
NaOH	2.271e-16	2.653e-16	-15.644	-15.576	0.067	
(0)						
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-56.624	-56.557	0.067	
31.90						
S(-2)	2.442e-25					
HS-	2.404e-25	1.434e-25	-24.619	-24.843	-0.224	
22.07						
H2S	3.779e-27	4.413e-27	-26.423	-26.355	0.067	
37.22						
S-2	7.360e-29	1.334e-29	-28.133	-28.875	-0.742	
(0)						
S(6)	1.100e-02					
SO4-2	4.493e-03	7.653e-04	-2.347	-3.116	-0.769	
19.80						
MgSO4	3.336e-03	3.896e-03	-2.477	-2.409	0.067	
6.56						
NaSO4-	2.082e-03	1.384e-03	-2.682	-2.859	-0.177	
20.38						
CaSO4	1.089e-03	1.272e-03	-2.963	-2.896	0.067	
8.21						
HSO4-	1.155e-09	8.503e-10	-8.938	-9.070	-0.133	
42.08						
CaHSO4+	1.104e-10	8.129e-11	-9.957	-10.090	-0.133	
(0)						

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

Phase	SI**	log IAP	log K(323 K, 11 atm)	
Anhydrite	-0.65	-5.22	-4.57	CaSO4
Aragonite	1.27	-7.26	-8.53	CaCO3
Calcite	1.39	-7.26	-8.65	CaCO3
CH4(g)	-24.76	-27.72	-2.97	CH4
CO2(g)	-3.37	-5.09	-1.72	CO2
Dolomite	3.27	-14.33	-17.61	CaMg(CO3)2
Gypsum	-0.62	-5.24	-4.61	CaSO4:2H2O
H2(g)	-11.06	-14.20	-3.14	H2
H2O(g)	-0.92	-0.01	0.91	H2O
H2S(g)	-25.09	-33.04	-7.95	H2S
Halite	-2.55	-0.96	1.59	NaCl
O2(g)	-53.52	-56.56	-3.04	O2
Sulfur	-19.74	-15.41	4.34	S

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.517 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=55.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=55.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 55
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg

REACTION_PRESSURE 1
10.89

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance (µS/cm, 55°C)	=	84902
Density (g/cm³)	=	1.00970
Volume (L)	=	1.02431
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.735e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.768e-03
Total CO2 (mol/kg)	=	1.768e-03
Temperature (°C)	=	55.00
Electrical balance (eq)	=	1.460e-02
Percent error, 100*(Cat- An)/(Cat+ An)	=	1.23
Iterations	=	8
Total H	=	1.110138e+02
Total O	=	5.555565e+01

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

mole V Species cm³/mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.917e-05	1.138e-05	-4.717	-4.944	-0.226	-
2.14 H+	8.472e-09	6.310e-09	-8.072	-8.200	-0.128	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.28 C(4)	1.768e-03					
HCO3-	9.003e-04	5.963e-04	-3.046	-3.224	-0.179	
27.94						

NaCO3-	2.050e-04	1.504e-04	-3.688	-3.823	-0.134	
4.60						
CaCO3	1.666e-04	1.946e-04	-3.778	-3.711	0.067	-
14.52						
MgHCO3+	1.660e-04	1.020e-04	-3.780	-3.992	-0.212	
6.33						
CaHCO3+	1.126e-04	7.653e-05	-3.948	-4.116	-0.168	
10.75						
MgCO3	1.006e-04	1.174e-04	-3.998	-3.930	0.067	-
17.10						
NaHCO3	7.639e-05	8.921e-05	-4.117	-4.050	0.067	
1.80						
CO3-2	3.418e-05	6.582e-06	-4.466	-5.182	-0.715	-
2.40						
CO2	6.347e-06	7.412e-06	-5.197	-5.130	0.067	
35.92						
(CO2) 2	1.990e-12	2.324e-12	-11.701	-11.634	0.067	
71.84						
Ca	3.500e-02					
Ca+2	3.366e-02	7.756e-03	-1.473	-2.110	-0.637	-
16.42						
CaSO4	1.064e-03	1.242e-03	-2.973	-2.906	0.067	
8.29						
CaCO3	1.666e-04	1.946e-04	-3.778	-3.711	0.067	-
14.52						
CaHCO3+	1.126e-04	7.653e-05	-3.948	-4.116	-0.168	
10.75						
CaOH+	2.727e-07	2.002e-07	-6.564	-6.699	-0.134	
(0)						
CaHSO4+	1.181e-10	8.666e-11	-9.928	-10.062	-0.134	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.520e-01	-0.243	-0.453	-0.211	
19.06						
H(0)	3.680e-28					
H2	1.840e-28	2.148e-28	-27.735	-27.668	0.067	
28.58						
Mg	4.800e-02					
Mg+2	4.411e-02	1.179e-02	-1.355	-1.928	-0.573	-
21.23						
MgSO4	3.508e-03	4.096e-03	-2.455	-2.388	0.067	
6.63						
MgHCO3+	1.660e-04	1.020e-04	-3.780	-3.992	-0.212	
6.33						
MgOH+	1.127e-04	7.804e-05	-3.948	-4.108	-0.159	
(0)						
MgCO3	1.006e-04	1.174e-04	-3.998	-3.930	0.067	-
17.10						
Na	4.450e-01					
Na+	4.427e-01	3.104e-01	-0.354	-0.508	-0.154	
0.43						
NaSO4-	2.050e-03	1.358e-03	-2.688	-2.867	-0.179	
20.15						
NaCO3-	2.050e-04	1.504e-04	-3.688	-3.823	-0.134	
4.60						
NaHCO3	7.639e-05	8.921e-05	-4.117	-4.050	0.067	
1.80						

NaOH	3.026e-16	3.533e-16	-15.519	-15.452	0.067
(0)					
O(0)	9.323e-29				
O2	4.662e-29	5.444e-29	-28.331	-28.264	0.067
32.16					
S(6)	1.100e-02				
SO4-2	4.379e-03	7.343e-04	-2.359	-3.134	-0.775
20.02					
MgSO4	3.508e-03	4.096e-03	-2.455	-2.388	0.067
6.63					
NaSO4-	2.050e-03	1.358e-03	-2.688	-2.867	-0.179
20.15					
CaSO4	1.064e-03	1.242e-03	-2.973	-2.906	0.067
8.29					
HSO4-	1.266e-09	9.293e-10	-8.898	-9.032	-0.134
42.23					
CaHSO4+	1.181e-10	8.666e-11	-9.928	-10.062	-0.134
(0)					

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

Phase	SI**	log IAP	log K(328 K,	1 atm)
Anhydrite	-0.60	-5.24	-4.64	CaSO4
Aragonite	1.29	-7.29	-8.59	CaCO3
Calcite	1.42	-7.29	-8.71	CaCO3
CO2(g)	-3.38	-5.13	-1.75	CO2
Dolomite	3.32	-14.40	-17.72	CaMg(CO3)2
Gypsum	-0.63	-5.26	-4.63	CaSO4:2H2O
H2(g)	-24.53	-27.67	-3.14	H2
H2O(g)	-0.82	-0.01	0.81	H2O
Halite	-2.55	-0.96	1.59	NaCl
O2(g)	-25.22	-28.26	-3.05	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
C	1.768e-03	1.768e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01

S 1.100e-02 1.100e-02

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

equilibrium
 pH = 8.197 Charge balance
 pe = -2.492 Adjusted to redox
 Specific Conductance (µS/cm, 55°C) = 84882
 Density (g/cm³) = 1.01012
 Volume (L) = 1.02389
 Activity of water = 0.981
 Ionic strength (mol/kgw) = 6.735e-01
 Mass of water (kg) = 1.000e+00
 Total alkalinity (eq/kg) = 2.400e-03
 Total CO2 (mol/kg) = 1.768e-03
 Temperature (°C) = 55.00
 Pressure (atm) = 10.89
 Electrical balance (eq) = 1.460e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
 Iterations = 14
 Total H = 1.110138e+02
 Total O = 5.555565e+01

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

mole V Species cm³/mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.918e-05	1.139e-05	-4.717	-4.943	-0.226	-
2.16						
H+	8.529e-09	6.353e-09	-8.069	-8.197	-0.128	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.27						
C(-4)	5.143e-31					
CH4	5.143e-31	6.006e-31	-30.289	-30.221	0.067	
37.68						
C(4)	1.768e-03					
HCO3-	8.989e-04	5.956e-04	-3.046	-3.225	-0.179	
27.95						
NaCO3-	2.051e-04	1.506e-04	-3.688	-3.822	-0.134	
4.68						
CaCO3	1.670e-04	1.951e-04	-3.777	-3.710	0.067	-
14.46						
MgHCO3+	1.659e-04	1.020e-04	-3.780	-3.992	-0.211	
6.36						
CaHCO3+	1.126e-04	7.652e-05	-3.949	-4.116	-0.168	
10.76						
MgCO3	1.007e-04	1.176e-04	-3.997	-3.930	0.067	-
17.02						
NaHCO3	7.706e-05	8.999e-05	-4.113	-4.046	0.067	
1.80						

CO3-2	3.426e-05	6.602e-06	-4.465	-5.180	-0.715	-
2.32						
CO2	6.322e-06	7.382e-06	-5.199	-5.132	0.067	
35.91						
(CO2)2	1.974e-12	2.305e-12	-11.705	-11.637	0.067	
71.82						
Ca	3.500e-02					
Ca+2	3.366e-02	7.763e-03	-1.473	-2.110	-0.637	-
16.35						
CaSO4	1.064e-03	1.243e-03	-2.973	-2.906	0.067	
8.31						
CaCO3	1.670e-04	1.951e-04	-3.777	-3.710	0.067	-
14.46						
CaHCO3+	1.126e-04	7.652e-05	-3.949	-4.116	-0.168	
10.76						
CaOH+	2.713e-07	1.991e-07	-6.567	-6.701	-0.134	
(0)						
CaHSO4+	1.192e-10	8.754e-11	-9.924	-10.058	-0.134	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.521e-01	-0.243	-0.453	-0.211	
19.06						
H(0)	3.564e-15					
H2	1.782e-15	2.081e-15	-14.749	-14.682	0.067	
28.58						
Mg	4.800e-02					
Mg+2	4.412e-02	1.180e-02	-1.355	-1.928	-0.573	-
21.16						
MgSO4	3.505e-03	4.092e-03	-2.455	-2.388	0.067	
6.65						
MgHCO3+	1.659e-04	1.020e-04	-3.780	-3.992	-0.211	
6.36						
MgOH+	1.119e-04	7.750e-05	-3.951	-4.111	-0.159	
(0)						
MgCO3	1.007e-04	1.176e-04	-3.997	-3.930	0.067	-
17.02						
Na	4.450e-01					
Na+	4.427e-01	3.105e-01	-0.354	-0.508	-0.154	
0.46						
NaSO4-	2.052e-03	1.360e-03	-2.688	-2.867	-0.179	
20.09						
NaCO3-	2.051e-04	1.506e-04	-3.688	-3.822	-0.134	
4.68						
NaHCO3	7.706e-05	8.999e-05	-4.113	-4.046	0.067	
1.80						
NaOH	3.026e-16	3.534e-16	-15.519	-15.452	0.067	
(0)						
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-54.312	-54.245	0.067	
32.14						
S(-2)	8.044e-28					
HS-	7.927e-28	4.708e-28	-27.101	-27.327	-0.226	
22.12						
H2S	1.143e-29	1.335e-29	-28.942	-28.875	0.067	
37.23						
S-2	3.269e-31	5.837e-32	-30.486	-31.234	-0.748	
(0)						

S(6)	1.100e-02					
SO4-2	4.379e-03	7.350e-04	-2.359	-3.134	-0.775	
19.99						
MgSO4	3.505e-03	4.092e-03	-2.455	-2.388	0.067	
6.65						
NaSO4-	2.052e-03	1.360e-03	-2.688	-2.867	-0.179	
20.09						
CaSO4	1.064e-03	1.243e-03	-2.973	-2.906	0.067	
8.31						
HSO4-	1.266e-09	9.290e-10	-8.898	-9.032	-0.134	
42.19						
CaHSO4+	1.192e-10	8.754e-11	-9.924	-10.058	-0.134	
(0)						

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

Phase	SI**	log IAP	log K(328 K, 11 atm)	
Anhydrite	-0.61	-5.24	-4.63	CaSO4
Aragonite	1.29	-7.29	-8.58	CaCO3
Calcite	1.41	-7.29	-8.70	CaCO3
CH4(g)	-27.24	-30.22	-2.98	CH4
CO2(g)	-3.38	-5.13	-1.75	CO2
Dolomite	3.31	-14.40	-17.71	CaMg(CO3)2
Gypsum	-0.63	-5.26	-4.63	CaSO4:2H2O
H2(g)	-11.54	-14.68	-3.14	H2
H2O(g)	-0.82	-0.01	0.81	H2O
H2S(g)	-27.58	-35.52	-7.95	H2S
Halite	-2.55	-0.96	1.59	NaCl
O2(g)	-51.19	-54.24	-3.05	O2
Sulfur	-21.70	-17.47	4.24	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

 Reading input data for simulation 2.

 End of Run after 0.144 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=60.pqi
 Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=60.pqo
 Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 60
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
10.89

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH = 8.200
pe = 4.000

Specific Conductance ($\mu\text{S}/\text{cm}$, 60°C) = 90709
 Density (g/cm^3) = 1.00716
 Volume (L) = 1.02689
 Activity of water = 0.981
 Ionic strength (mol/kgw) = $6.729\text{e-}01$
 Mass of water (kg) = $1.000\text{e+}00$
 Total carbon (mol/kg) = $1.679\text{e-}03$
 Total CO_2 (mol/kg) = $1.679\text{e-}03$
 Temperature ($^\circ\text{C}$) = 60.00
 Electrical balance (eq) = $1.460\text{e-}02$
 Percent error, $100 * (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = 1.24
 Iterations = 8
 Total H = $1.110138\text{e+}02$
 Total O = $5.555543\text{e+}01$

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

--

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm^3/mol						
OH-	$2.541\text{e-}05$	$1.501\text{e-}05$	-4.595	-4.824	-0.228	-
2.18						
H+	$8.493\text{e-}09$	$6.310\text{e-}09$	-8.071	-8.200	-0.129	
0.00						
H ₂ O	$5.551\text{e+}01$	$9.812\text{e-}01$	1.744	-0.008	0.000	
18.32						
C(4)	$1.679\text{e-}03$					
HCO ₃ -	$8.099\text{e-}04$	$5.345\text{e-}04$	-3.092	-3.272	-0.180	
27.97						
NaCO ₃ -	$2.323\text{e-}04$	$1.699\text{e-}04$	-3.634	-3.770	-0.136	
4.64						
CaCO ₃	$1.780\text{e-}04$	$2.078\text{e-}04$	-3.750	-3.682	0.067	-
14.51						
MgHCO ₃ +	$1.540\text{e-}04$	$9.418\text{e-}05$	-3.813	-4.026	-0.214	
6.36						
CaHCO ₃ +	$1.022\text{e-}04$	$6.921\text{e-}05$	-3.991	-4.160	-0.169	
10.82						
MgCO ₃	$9.846\text{e-}05$	$1.150\text{e-}04$	-4.007	-3.939	0.067	-
17.09						
NaHCO ₃	$6.663\text{e-}05$	$7.779\text{e-}05$	-4.176	-4.109	0.067	
1.80						
CO ₃ -2	$3.206\text{e-}05$	$6.084\text{e-}06$	-4.494	-5.216	-0.722	-
2.84						
CO ₂	$5.744\text{e-}06$	$6.707\text{e-}06$	-5.241	-5.173	0.067	
36.19						
(CO ₂) ₂	$1.822\text{e-}12$	$2.128\text{e-}12$	-11.739	-11.672	0.067	
72.38						
Ca	$3.500\text{e-}02$					
Ca+2	$3.368\text{e-}02$	$7.642\text{e-}03$	-1.473	-2.117	-0.644	-
16.44						
CaSO ₄	$1.038\text{e-}03$	$1.212\text{e-}03$	-2.984	-2.916	0.067	
8.37						
CaCO ₃	$1.780\text{e-}04$	$2.078\text{e-}04$	-3.750	-3.682	0.067	-
14.51						

CaHCO3+	1.022e-04	6.921e-05	-3.991	-4.160	-0.169	
10.82						
CaOH+	2.696e-07	1.972e-07	-6.569	-6.705	-0.136	
(0)						
CaHSO4+	1.280e-10	9.361e-11	-9.893	-10.029	-0.136	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.503e-01	-0.243	-0.456	-0.213	
19.00						
H(0)	3.534e-28					
H2	1.767e-28	2.063e-28	-27.753	-27.685	0.067	
28.58						
Mg	4.800e-02					
Mg+2	4.392e-02	1.157e-02	-1.357	-1.937	-0.579	-
21.38						
MgSO4	3.671e-03	4.286e-03	-2.435	-2.368	0.067	
6.72						
MgOH+	1.601e-04	1.105e-04	-3.796	-3.957	-0.161	
(0)						
MgHCO3+	1.540e-04	9.418e-05	-3.813	-4.026	-0.214	
6.36						
MgCO3	9.846e-05	1.150e-04	-4.007	-3.939	0.067	-
17.09						
Na	4.450e-01					
Na+	4.427e-01	3.090e-01	-0.354	-0.510	-0.156	
0.54						
NaSO4-	2.019e-03	1.332e-03	-2.695	-2.875	-0.180	
19.82						
NaCO3-	2.323e-04	1.699e-04	-3.634	-3.770	-0.136	
4.64						
NaHCO3	6.663e-05	7.779e-05	-4.176	-4.109	0.067	
1.80						
NaOH	3.973e-16	4.639e-16	-15.401	-15.334	0.067	
(0)						
O(0)	2.074e-27					
O2	1.037e-27	1.211e-27	-26.984	-26.917	0.067	
32.38						
S(6)	1.100e-02					
SO4-2	4.271e-03	7.054e-04	-2.369	-3.152	-0.782	
20.15						
MgSO4	3.671e-03	4.286e-03	-2.435	-2.368	0.067	
6.72						
NaSO4-	2.019e-03	1.332e-03	-2.695	-2.875	-0.180	
19.82						
CaSO4	1.038e-03	1.212e-03	-2.984	-2.916	0.067	
8.37						
HSO4-	1.393e-09	1.019e-09	-8.856	-8.992	-0.136	
42.31						
CaHSO4+	1.280e-10	9.361e-11	-9.893	-10.029	-0.136	
(0)						

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

Phase	SI**	log IAP	log K(333 K,	1 atm)
Anhydrite	-0.56	-5.27	-4.71	CaSO4

Aragonite	1.30	-7.33	-8.64	CaCO3
Calcite	1.43	-7.33	-8.76	CaCO3
CO2(g)	-3.39	-5.17	-1.78	CO2
Dolomite	3.33	-14.49	-17.82	CaMg(CO3)2
Gypsum	-0.63	-5.28	-4.65	CaSO4:2H2O
H2(g)	-24.55	-27.69	-3.14	H2
H2O(g)	-0.72	-0.01	0.71	H2O
Halite	-2.56	-0.97	1.60	NaCl
O2(g)	-23.85	-26.92	-3.06	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
 Using pressure 1.

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

--

Elements	Molality	Moles
C	1.679e-03	1.679e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	8.197	Charge balance
	pe =	7.307	Adjusted to redox
equilibrium			
	Specific Conductance (µS/cm, 60°C)	=	90682
	Density (g/cm³)	=	1.00758
	Volume (L)	=	1.02646
	Activity of water	=	0.981
	Ionic strength (mol/kgw)	=	6.729e-01
	Mass of water (kg)	=	1.000e+00
	Total alkalinity (eq/kg)	=	2.400e-03
	Total CO2 (mol/kg)	=	1.679e-03
	Temperature (°C)	=	60.00
	Pressure (atm)	=	10.89
	Electrical balance (eq)	=	1.460e-02
Percent error, 100*(Cat- An)/(Cat+ An)		=	1.24
	Iterations	=	10
	Total H	=	1.110138e+02
	Total O	=	5.555543e+01

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

--

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	2.543e-05	1.503e-05	-4.595	-4.823	-0.228	-
2.21						
H+	8.545e-09	6.349e-09	-8.068	-8.197	-0.129	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.32						
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-109.334	-109.267	0.067	
38.02						
C(4)	1.679e-03					
HCO3-	8.085e-04	5.337e-04	-3.092	-3.273	-0.180	
27.98						
NaCO3-	2.325e-04	1.701e-04	-3.633	-3.769	-0.136	
4.72						
CaCO3	1.784e-04	2.083e-04	-3.749	-3.681	0.067	-
14.45						
MgHCO3+	1.539e-04	9.414e-05	-3.813	-4.026	-0.213	
6.38						
CaHCO3+	1.021e-04	6.919e-05	-3.991	-4.160	-0.169	
10.84						
MgCO3	9.864e-05	1.152e-04	-4.006	-3.939	0.067	-
17.02						
NaHCO3	6.719e-05	7.845e-05	-4.173	-4.105	0.067	
1.80						
CO3-2	3.214e-05	6.105e-06	-4.493	-5.214	-0.721	-
2.76						
CO2	5.716e-06	6.674e-06	-5.243	-5.176	0.067	
36.18						
(CO2)2	1.805e-12	2.107e-12	-11.744	-11.676	0.067	
72.36						
Ca	3.500e-02					
Ca+2	3.368e-02	7.649e-03	-1.473	-2.116	-0.644	-
16.37						
CaSO4	1.039e-03	1.213e-03	-2.984	-2.916	0.067	
8.40						
CaCO3	1.784e-04	2.083e-04	-3.749	-3.681	0.067	-
14.45						
CaHCO3+	1.021e-04	6.919e-05	-3.991	-4.160	-0.169	
10.84						
CaOH+	2.683e-07	1.963e-07	-6.571	-6.707	-0.136	
(0)						
CaHSO4+	1.292e-10	9.450e-11	-9.889	-10.025	-0.136	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.504e-01	-0.243	-0.455	-0.213	
19.00						
H(0)	8.595e-35					
H2	4.298e-35	5.018e-35	-34.367	-34.299	0.067	
28.58						

Mg	4.800e-02					
Mg+2	4.392e-02	1.158e-02	-1.357	-1.936	-0.579	-
21.31						
MgSO4	3.668e-03	4.283e-03	-2.436	-2.368	0.067	
6.74						
MgOH+	1.590e-04	1.098e-04	-3.798	-3.959	-0.161	
(0)						
MgHCO3+	1.539e-04	9.414e-05	-3.813	-4.026	-0.213	
6.38						
MgCO3	9.864e-05	1.152e-04	-4.006	-3.939	0.067	-
17.02						
Na	4.450e-01					
Na+	4.427e-01	3.091e-01	-0.354	-0.510	-0.156	
0.57						
NaSO4-	2.022e-03	1.335e-03	-2.694	-2.875	-0.180	
19.76						
NaCO3-	2.325e-04	1.701e-04	-3.633	-3.769	-0.136	
4.72						
NaHCO3	6.719e-05	7.845e-05	-4.173	-4.105	0.067	
1.80						
NaOH	3.977e-16	4.644e-16	-15.400	-15.333	0.067	
(0)						
O(0)	3.440e-14					
O2	1.720e-14	2.008e-14	-13.764	-13.697	0.067	
32.36						
S(-2)	0.000e+00					
HS-	0.000e+00	0.000e+00	-106.118	-106.347	-0.228	
22.13						
H2S	0.000e+00	0.000e+00	-107.992	-107.925	0.067	
37.24						
S-2	0.000e+00	0.000e+00	-109.377	-110.132	-0.755	
(0)						
S(6)	1.100e-02					
SO4-2	4.272e-03	7.061e-04	-2.369	-3.151	-0.782	
20.12						
MgSO4	3.668e-03	4.283e-03	-2.436	-2.368	0.067	
6.74						
NaSO4-	2.022e-03	1.335e-03	-2.694	-2.875	-0.180	
19.76						
CaSO4	1.039e-03	1.213e-03	-2.984	-2.916	0.067	
8.40						
HSO4-	1.392e-09	1.018e-09	-8.856	-8.992	-0.136	
42.28						
CaHSO4+	1.292e-10	9.450e-11	-9.889	-10.025	-0.136	
(0)						

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

Phase	SI**	log IAP	log K(333 K, 11 atm)	
Anhydrite	-0.57	-5.27	-4.70	CaSO4
Aragonite	1.30	-7.33	-8.63	CaCO3
Calcite	1.42	-7.33	-8.75	CaCO3
CH4 (g)	-106.27	-109.27	-3.00	CH4
CO2 (g)	-3.39	-5.18	-1.79	CO2
Dolomite	3.32	-14.48	-17.80	CaMg (CO3) 2

Gypsum	-0.64	-5.28	-4.65	CaSO4:2H2O
H2 (g)	-31.16	-34.30	-3.14	H2
H2O (g)	-0.71	-0.01	0.71	H2O
H2S (g)	-106.60	-114.54	-7.94	H2S
Halite	-2.56	-0.97	1.60	NaCl
O2 (g)	-10.63	-13.70	-3.07	O2
Sulfur	-81.06	-76.92	4.14	S

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.598 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=70.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=70.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 70
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1

```

Ca      35
Mg      48
Na     445
S(6)   11
Alkalinity 2.4 as HCO3-
Cl     572
water  1 # kg
REACTION PRESSURE 1
10.89

```

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

```

pH = 8.200
pe = 4.000
Specific Conductance (µS/cm, 70°C) = 102419
Density (g/cm³) = 1.00168
Volume (L) = 1.03249
Activity of water = 0.981
Ionic strength (mol/kgw) = 6.717e-01
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 1.470e-03
Total CO2 (mol/kg) = 1.470e-03
Temperature (°C) = 70.00
Electrical balance (eq) = 1.460e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.24
Iterations = 8
Total H = 1.110137e+02
Total O = 5.555498e+01

```

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

mole V Species cm ³ /mol	Molality	Activity	Log	Log	Log	Gamma
			Molality	Activity	Gamma	
OH- 2.36	4.295e-05	2.513e-05	-4.367	-4.600	-0.233	-

H+	8.539e-09	6.310e-09	-8.069	-8.200	-0.131	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.43						
C(4)	1.470e-03					
HCO3-	6.292e-04	4.121e-04	-3.201	-3.385	-0.184	
27.95						
NaCO3-	2.743e-04	1.992e-04	-3.562	-3.701	-0.139	
4.55						
CaCO3	1.900e-04	2.218e-04	-3.721	-3.654	0.067	-
14.49						
MgHCO3+	1.281e-04	7.763e-05	-3.892	-4.110	-0.218	
6.38						
MgCO3	8.813e-05	1.029e-04	-4.055	-3.988	0.067	-
17.09						
CaHCO3+	8.071e-05	5.427e-05	-4.093	-4.265	-0.172	
10.94						
NaHCO3	4.871e-05	5.686e-05	-4.312	-4.245	0.067	
1.80						
CO3-2	2.644e-05	4.863e-06	-4.578	-5.313	-0.735	-
3.99						
CO2	4.619e-06	5.391e-06	-5.335	-5.268	0.067	
36.77						
(CO2)2	1.444e-12	1.686e-12	-11.840	-11.773	0.067	
73.54						
Ca	3.500e-02					
Ca+2	3.374e-02	7.407e-03	-1.472	-2.130	-0.659	-
16.52						
CaSO4	9.863e-04	1.151e-03	-3.006	-2.939	0.067	
8.53						
CaCO3	1.900e-04	2.218e-04	-3.721	-3.654	0.067	-
14.49						
CaHCO3+	8.071e-05	5.427e-05	-4.093	-4.265	-0.172	
10.94						
CaOH+	2.632e-07	1.912e-07	-6.580	-6.719	-0.139	
(0)						
CaHSO4+	1.516e-10	1.101e-10	-9.819	-9.958	-0.139	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.469e-01	-0.243	-0.460	-0.217	
18.80						
H(0)	3.272e-28					
H2	1.636e-28	1.910e-28	-27.786	-27.719	0.067	
28.58						
Mg	4.800e-02					
Mg+2	4.349e-02	1.111e-02	-1.362	-1.954	-0.593	-
21.70						
MgSO4	3.980e-03	4.646e-03	-2.400	-2.333	0.067	
6.87						
MgOH+	3.123e-04	2.141e-04	-3.505	-3.669	-0.164	
(0)						
MgHCO3+	1.281e-04	7.763e-05	-3.892	-4.110	-0.218	
6.38						
MgCO3	8.813e-05	1.029e-04	-4.055	-3.988	0.067	-
17.09						
Na	4.450e-01					

Na+	4.427e-01	3.061e-01	-0.354	-0.514	-0.160
0.72					
NaSO4-	1.957e-03	1.281e-03	-2.708	-2.892	-0.184
19.01					
NaCO3-	2.743e-04	1.992e-04	-3.562	-3.701	-0.139
4.55					
NaHCO3	4.871e-05	5.686e-05	-4.312	-4.245	0.067
1.80					
NaOH	6.590e-16	7.692e-16	-15.181	-15.114	0.067
(0)					
O(0)	7.829e-25				
O2	3.914e-25	4.569e-25	-24.407	-24.340	0.067
32.79					
S(6)	1.100e-02				
SO4-2	4.077e-03	6.518e-04	-2.390	-3.186	-0.796
20.21					
MgSO4	3.980e-03	4.646e-03	-2.400	-2.333	0.067
6.87					
NaSO4-	1.957e-03	1.281e-03	-2.708	-2.892	-0.184
19.01					
CaSO4	9.863e-04	1.151e-03	-3.006	-2.939	0.067
8.53					
HSO4-	1.702e-09	1.236e-09	-8.769	-8.908	-0.139
42.41					
CaHSO4+	1.516e-10	1.101e-10	-9.819	-9.958	-0.139
(0)					

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

Phase	SI**	log IAP	log K(343 K,	1 atm)
Anhydrite	-0.48	-5.32	-4.84	CaSO4
Aragonite	1.31	-7.44	-8.75	CaCO3
Calcite	1.42	-7.44	-8.87	CaCO3
CO2(g)	-3.42	-5.27	-1.85	CO2
Dolomite	3.29	-14.71	-18.00	CaMg(CO3)2
Gypsum	-0.64	-5.33	-4.69	CaSO4:2H2O
H2(g)	-24.58	-27.72	-3.14	H2
H2O(g)	-0.52	-0.01	0.51	H2O
Halite	-2.58	-0.97	1.60	NaCl
O2(g)	-21.25	-24.34	-3.09	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
C	1.470e-03	1.470e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	8.198	Charge balance
	pe =	-2.327	Adjusted to redox
equilibrium			
Specific Conductance ($\mu\text{S}/\text{cm}$, 70°C)	=	102377	
Density (g/cm^3)	=	1.00211	
Volume (L)	=	1.03205	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.718e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	2.400e-03	
Total CO2 (mol/kg)	=	1.470e-03	
Temperature (°C)	=	70.00	
Pressure (atm)	=	10.89	
Electrical balance (eq)	=	1.460e-02	
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.24	
Iterations	=	14	
Total H	=	1.110137e+02	
Total O	=	5.555498e+01	

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	4.305e-05	2.519e-05	-4.366	-4.599	-0.233	-
2.40						
H+	8.578e-09	6.339e-09	-8.067	-8.198	-0.131	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.42						
C(-4)	2.952e-34					
CH4	2.952e-34	3.446e-34	-33.530	-33.463	0.067	
38.72						
C(4)	1.470e-03					
HCO3-	6.278e-04	4.112e-04	-3.202	-3.386	-0.184	
27.96						
NaCO3-	2.748e-04	1.996e-04	-3.561	-3.700	-0.139	
4.63						
CaCO3	1.907e-04	2.225e-04	-3.720	-3.653	0.067	-
14.43						

MgHCO3+	1.279e-04	7.755e-05	-3.893	-4.110	-0.217	
6.40						
MgCO3	8.835e-05	1.031e-04	-4.054	-3.987	0.067	-
17.02						
CaHCO3+	8.061e-05	5.422e-05	-4.094	-4.266	-0.172	
10.96						
NaHCO3	4.908e-05	5.729e-05	-4.309	-4.242	0.067	
1.80						
CO3-2	2.653e-05	4.885e-06	-4.576	-5.311	-0.735	-
3.90						
CO2	4.586e-06	5.354e-06	-5.339	-5.271	0.067	
36.75						
(CO2) 2	1.424e-12	1.663e-12	-11.846	-11.779	0.067	
73.50						
Ca	3.500e-02					
Ca+2	3.374e-02	7.415e-03	-1.472	-2.130	-0.658	-
16.45						
CaSO4	9.865e-04	1.152e-03	-3.006	-2.939	0.067	
8.55						
CaCO3	1.907e-04	2.225e-04	-3.720	-3.653	0.067	-
14.43						
CaHCO3+	8.061e-05	5.422e-05	-4.094	-4.266	-0.172	
10.96						
CaOH+	2.624e-07	1.906e-07	-6.581	-6.720	-0.139	
(0)						
CaHSO4+	1.528e-10	1.110e-10	-9.816	-9.955	-0.139	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.470e-01	-0.243	-0.460	-0.217	
18.80						
H(0)	1.473e-15					
H2	7.364e-16	8.596e-16	-15.133	-15.066	0.067	
28.57						
Mg	4.800e-02					
Mg+2	4.350e-02	1.112e-02	-1.362	-1.954	-0.592	-
21.62						
MgSO4	3.976e-03	4.641e-03	-2.401	-2.333	0.067	
6.89						
MgOH+	3.107e-04	2.131e-04	-3.508	-3.671	-0.164	
(0)						
MgHCO3+	1.279e-04	7.755e-05	-3.893	-4.110	-0.217	
6.40						
MgCO3	8.835e-05	1.031e-04	-4.054	-3.987	0.067	-
17.02						
Na	4.450e-01					
Na+	4.427e-01	3.062e-01	-0.354	-0.514	-0.160	
0.75						
NaSO4-	1.960e-03	1.284e-03	-2.708	-2.891	-0.184	
18.96						
NaCO3-	2.748e-04	1.996e-04	-3.561	-3.700	-0.139	
4.63						
NaHCO3	4.908e-05	5.729e-05	-4.309	-4.242	0.067	
1.80						
NaOH	6.605e-16	7.710e-16	-15.180	-15.113	0.067	
(0)						
O(0)	0.000e+00					

O2	0.000e+00	0.000e+00	-49.722	-49.655	0.067
32.76					
S(-2)	5.974e-31				
HS-	5.899e-31	3.452e-31	-30.229	-30.462	-0.233
22.08					
H2S	6.979e-33	8.146e-33	-32.156	-32.089	0.067
37.25					
S-2	5.668e-34	9.650e-35	-33.247	-34.015	-0.769
(0)					
S(6)	1.100e-02				
SO4-2	4.077e-03	6.525e-04	-2.390	-3.185	-0.796
20.19					
MgSO4	3.976e-03	4.641e-03	-2.401	-2.333	0.067
6.89					
NaSO4-	1.960e-03	1.284e-03	-2.708	-2.891	-0.184
18.96					
CaSO4	9.865e-04	1.152e-03	-3.006	-2.939	0.067
8.55					
HSO4-	1.698e-09	1.234e-09	-8.770	-8.909	-0.139
42.38					
CaHSO4+	1.528e-10	1.110e-10	-9.816	-9.955	-0.139
(0)					

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

Phase	SI**	log IAP	log K(343 K, 11 atm)	
Anhydrite	-0.48	-5.32	-4.83	CaSO4
Aragonite	1.30	-7.44	-8.74	CaCO3
Calcite	1.42	-7.44	-8.86	CaCO3
CH4(g)	-30.45	-33.46	-3.01	CH4
CO2(g)	-3.42	-5.27	-1.85	CO2
Dolomite	3.27	-14.71	-17.98	CaMg(CO3)2
Gypsum	-0.65	-5.33	-4.69	CaSO4:2H2O
H2(g)	-11.93	-15.07	-3.14	H2
H2O(g)	-0.52	-0.01	0.51	H2O
H2S(g)	-30.72	-38.66	-7.94	H2S
Halite	-2.58	-0.97	1.60	NaCl
O2(g)	-46.56	-49.65	-3.09	O2
Sulfur	-24.31	-20.35	3.96	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

 Reading input data for simulation 2.

 End of Run after 0.14 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=80.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=80.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 80
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
10.89

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01

Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

--

	pH	=	8.200
	pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 80°C)		=	114163
Density (g/cm^3)		=	0.99572
Volume (L)		=	1.03866
Activity of water		=	0.981
Ionic strength (mol/kgw)		=	6.706e-01
Mass of water (kg)		=	1.000e+00
Total carbon (mol/kg)		=	1.198e-03
Total CO2 (mol/kg)		=	1.198e-03
Temperature (°C)		=	80.00
Electrical balance (eq)		=	1.460e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$		=	1.24
	Iterations	=	9
	Total H	=	1.110137e+02
	Total O	=	5.555446e+01

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

--

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm^3/mol						
OH-	6.927e-05	4.009e-05	-4.159	-4.397	-0.238	-
2.66						
H+	8.588e-09	6.310e-09	-8.066	-8.200	-0.134	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.54						
C(4)	1.198e-03					
HCO3-	4.509e-04	2.928e-04	-3.346	-3.533	-0.187	
27.82						
NaCO3-	2.831e-04	2.041e-04	-3.548	-3.690	-0.142	
4.25						
CaCO3	1.797e-04	2.097e-04	-3.745	-3.678	0.067	-
14.47						
MgHCO3+	9.900e-05	5.940e-05	-4.004	-4.226	-0.222	
6.35						
MgCO3	7.023e-05	8.196e-05	-4.153	-4.086	0.067	-
17.08						
CaHCO3+	5.928e-05	3.956e-05	-4.227	-4.403	-0.176	
11.03						
NaHCO3	3.289e-05	3.838e-05	-4.483	-4.416	0.067	
1.80						
CO3-2	1.953e-05	3.476e-06	-4.709	-5.459	-0.750	-
5.50						
CO2	3.516e-06	4.103e-06	-5.454	-5.387	0.067	
37.40						

(CO2)2	1.001e-12	1.168e-12	-12.000	-11.933	0.067	
74.80						
Ca	3.500e-02					
Ca+2	3.383e-02	7.168e-03	-1.471	-2.145	-0.674	-
16.65						
CaSO4	9.344e-04	1.090e-03	-3.029	-2.962	0.067	
8.66						
CaCO3	1.797e-04	2.097e-04	-3.745	-3.678	0.067	-
14.47						
CaHCO3+	5.928e-05	3.956e-05	-4.227	-4.403	-0.176	
11.03						
CaOH+	2.567e-07	1.850e-07	-6.591	-6.733	-0.142	
(0)						
CaHSO4+	1.815e-10	1.308e-10	-9.741	-9.883	-0.142	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.432e-01	-0.243	-0.464	-0.222	
18.51						
H(0)	3.042e-28					
H2	1.521e-28	1.775e-28	-27.818	-27.751	0.067	
28.57						
Mg	4.800e-02					
Mg+2	4.299e-02	1.062e-02	-1.367	-1.974	-0.607	-
22.04						
MgSO4	4.259e-03	4.970e-03	-2.371	-2.304	0.067	
7.00						
MgOH+	5.832e-04	3.970e-04	-3.234	-3.401	-0.167	
(0)						
MgHCO3+	9.900e-05	5.940e-05	-4.004	-4.226	-0.222	
6.35						
MgCO3	7.023e-05	8.196e-05	-4.153	-4.086	0.067	-
17.08						
Na	4.450e-01					
Na+	4.428e-01	3.031e-01	-0.354	-0.518	-0.165	
0.88						
NaSO4-	1.896e-03	1.231e-03	-2.722	-2.910	-0.187	
18.01						
NaCO3-	2.831e-04	2.041e-04	-3.548	-3.690	-0.142	
4.25						
NaHCO3	3.289e-05	3.838e-05	-4.483	-4.416	0.067	
1.80						
NaOH	1.041e-15	1.215e-15	-14.982	-14.915	0.067	
(0)						
O(0)	2.111e-22					
O2	1.056e-22	1.232e-22	-21.976	-21.909	0.067	
33.17						
S(6)	1.100e-02					
MgSO4	4.259e-03	4.970e-03	-2.371	-2.304	0.067	
7.00						
SO4-2	3.911e-03	6.039e-04	-2.408	-3.219	-0.811	
20.04						
NaSO4-	1.896e-03	1.231e-03	-2.722	-2.910	-0.187	
18.01						
CaSO4	9.344e-04	1.090e-03	-3.029	-2.962	0.067	
8.66						
HSO4-	2.106e-09	1.518e-09	-8.676	-8.819	-0.142	
42.42						

CaHSO4+ 1.815e-10 1.308e-10 -9.741 -9.883 -0.142
 (0)

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

--

Phase	SI**	log IAP	log K(353 K,	1 atm)
Anhydrite	-0.39	-5.36	-4.98	CaSO4
Aragonite	1.27	-7.60	-8.88	CaCO3
Calcite	1.39	-7.60	-8.99	CaCO3
CO2(g)	-3.49	-5.39	-1.90	CO2
Dolomite	3.13	-15.04	-18.17	CaMg(CO3)2
Gypsum	-0.64	-5.38	-4.74	CaSO4:2H2O
H2(g)	-24.62	-27.75	-3.13	H2
H2O(g)	-0.34	-0.01	0.33	H2O
Halite	-2.59	-0.98	1.61	NaCl
O2(g)	-18.80	-21.91	-3.11	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
 Using pressure 1.

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

--

Elements	Molality	Moles
C	1.198e-03	1.198e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	8.199	Charge balance
	pe =	-2.936	Adjusted to redox
equilibrium			
	Specific Conductance (µS/cm, 80°C)	=	114105
	Density (g/cm³)	=	0.99616
	Volume (L)	=	1.03820
	Activity of water	=	0.981
	Ionic strength (mol/kgw)	=	6.706e-01
	Mass of water (kg)	=	1.000e+00
	Total alkalinity (eq/kg)	=	2.400e-03
	Total CO2 (mol/kg)	=	1.198e-03

Temperature (°C) = 80.00
 Pressure (atm) = 10.89
 Electrical balance (eq) = 1.460e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.24
 Iterations = 10
 Total H = 1.110137e+02
 Total O = 5.555446e+01

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

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm ³ /mol						
OH-	6.953e-05	4.026e-05	-4.158	-4.395	-0.237	-
2.70						
H+	8.613e-09	6.329e-09	-8.065	-8.199	-0.134	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.53						
C(-4)	1.231e-30					
CH4	1.231e-30	1.437e-30	-29.910	-29.843	0.067	
39.44						
C(4)	1.198e-03					
HCO3-	4.494e-04	2.920e-04	-3.347	-3.535	-0.187	
27.84						
NaCO3-	2.838e-04	2.046e-04	-3.547	-3.689	-0.142	
4.34						
CaCO3	1.804e-04	2.105e-04	-3.744	-3.677	0.067	-
14.41						
MgHCO3+	9.878e-05	5.928e-05	-4.005	-4.227	-0.222	
6.38						
MgCO3	7.043e-05	8.219e-05	-4.152	-4.085	0.067	-
17.02						
CaHCO3+	5.916e-05	3.948e-05	-4.228	-4.404	-0.176	
11.05						
NaHCO3	3.310e-05	3.863e-05	-4.480	-4.413	0.067	
1.80						
CO3-2	1.961e-05	3.494e-06	-4.707	-5.457	-0.749	-
5.40						
CO2	3.483e-06	4.064e-06	-5.458	-5.391	0.067	
37.38						
(CO2)2	9.820e-13	1.146e-12	-12.008	-11.941	0.067	
74.76						
Ca	3.500e-02					
Ca+2	3.383e-02	7.176e-03	-1.471	-2.144	-0.673	-
16.59						
CaSO4	9.346e-04	1.091e-03	-3.029	-2.962	0.067	
8.67						
CaCO3	1.804e-04	2.105e-04	-3.744	-3.677	0.067	-
14.41						
CaHCO3+	5.916e-05	3.948e-05	-4.228	-4.404	-0.176	
11.05						
CaOH+	2.563e-07	1.847e-07	-6.591	-6.733	-0.142	
(0)						

CaHSO4+	1.826e-10	1.316e-10	-9.738	-9.881	-0.142	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.433e-01	-0.243	-0.464	-0.222	
18.51						
H(0)	2.257e-14					
H2	1.129e-14	1.317e-14	-13.947	-13.880	0.067	
28.57						
Mg	4.800e-02					
Mg+2	4.299e-02	1.063e-02	-1.367	-1.973	-0.607	-
21.97						
MgSO4	4.255e-03	4.966e-03	-2.371	-2.304	0.067	
7.02						
MgOH+	5.813e-04	3.958e-04	-3.236	-3.403	-0.167	
(0)						
MgHCO3+	9.878e-05	5.928e-05	-4.005	-4.227	-0.222	
6.38						
MgCO3	7.043e-05	8.219e-05	-4.152	-4.085	0.067	-
17.02						
Na	4.450e-01					
Na+	4.428e-01	3.032e-01	-0.354	-0.518	-0.164	
0.91						
NaSO4-	1.900e-03	1.234e-03	-2.721	-2.909	-0.187	
17.96						
NaCO3-	2.838e-04	2.046e-04	-3.547	-3.689	-0.142	
4.34						
NaHCO3	3.310e-05	3.863e-05	-4.480	-4.413	0.067	
1.80						
NaOH	1.045e-15	1.220e-15	-14.981	-14.914	0.067	
(0)						
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-49.725	-49.658	0.067	
33.14						
S(-2)	3.391e-27					
HS-	3.349e-27	1.939e-27	-26.475	-26.712	-0.237	
21.95						
H2S	3.637e-29	4.244e-29	-28.439	-28.372	0.067	
37.27						
S-2	5.455e-30	8.970e-31	-29.263	-30.047	-0.784	
(0)						
S(6)	1.100e-02					
MgSO4	4.255e-03	4.966e-03	-2.371	-2.304	0.067	
7.02						
SO4-2	3.911e-03	6.045e-04	-2.408	-3.219	-0.811	
20.03						
NaSO4-	1.900e-03	1.234e-03	-2.721	-2.909	-0.187	
17.96						
CaSO4	9.346e-04	1.091e-03	-3.029	-2.962	0.067	
8.67						
HSO4-	2.098e-09	1.513e-09	-8.678	-8.820	-0.142	
42.39						
CaHSO4+	1.826e-10	1.316e-10	-9.738	-9.881	-0.142	
(0)						

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

Phase	SI**	log IAP	log K(353 K,	11 atm)	
Anhydrite	-0.39	-5.36	-4.97		CaSO4
Aragonite	1.27	-7.60	-8.87		CaCO3
Calcite	1.38	-7.60	-8.98		CaCO3
CH4(g)	-26.82	-29.84	-3.02		CH4
CO2(g)	-3.49	-5.39	-1.90		CO2
Dolomite	3.12	-15.03	-18.15		CaMg(CO3)2
Gypsum	-0.65	-5.38	-4.73		CaSO4:2H2O
H2(g)	-10.75	-13.88	-3.13		H2
H2O(g)	-0.34	-0.01	0.33		H2O
H2S(g)	-26.98	-34.91	-7.93		H2S
Halite	-2.59	-0.98	1.61		NaCl
O2(g)	-46.55	-49.66	-3.11		O2
Sulfur	-21.64	-17.85	3.79		S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.165 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=90.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=90.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 90
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
10.89

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 90°C)	=	125834
Density (g/cm^3)	=	0.98930
Volume (L)	=	1.04539
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.694e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	8.224e-04
Total CO2 (mol/kg)	=	8.224e-04
Temperature (°C)	=	90.00
Electrical balance (eq)	=	1.460e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.24
Iterations	=	8
Total H	=	1.110140e+02
Total O	=	5.555383e+01

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

--

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.070e-04	6.123e-05	-3.971	-4.213	-0.243	-
3.06						
H+	8.642e-09	6.310e-09	-8.063	-8.200	-0.137	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.66						
C(4)	8.224e-04					
HCO3-	2.717e-04	1.749e-04	-3.566	-3.757	-0.191	
27.60						
NaCO3-	2.342e-04	1.674e-04	-3.630	-3.776	-0.146	
3.76						
CaCO3	1.363e-04	1.590e-04	-3.866	-3.799	0.067	-
14.45						
MgHCO3+	6.461e-05	3.835e-05	-4.190	-4.416	-0.227	
6.29						
MgCO3	4.550e-05	5.309e-05	-4.342	-4.275	0.067	-
17.08						
CaHCO3+	3.731e-05	2.469e-05	-4.428	-4.607	-0.179	
11.09						
NaHCO3	1.869e-05	2.181e-05	-4.728	-4.661	0.067	
1.80						
CO3-2	1.183e-05	2.031e-06	-4.927	-5.692	-0.765	-
7.36						
CO2	2.302e-06	2.686e-06	-5.638	-5.571	0.067	
38.10						
(CO2)2	5.015e-13	5.850e-13	-12.300	-12.233	0.067	
76.21						
Ca	3.500e-02					
Ca+2	3.394e-02	6.926e-03	-1.469	-2.160	-0.690	-
16.84						
CaSO4	8.846e-04	1.032e-03	-3.053	-2.986	0.067	
8.76						
CaCO3	1.363e-04	1.590e-04	-3.866	-3.799	0.067	-
14.45						
CaHCO3+	3.731e-05	2.469e-05	-4.428	-4.607	-0.179	
11.09						
CaOH+	2.501e-07	1.788e-07	-6.602	-6.748	-0.146	
(0)						
CaHSO4+	2.198e-10	1.571e-10	-9.658	-9.804	-0.146	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.393e-01	-0.243	-0.469	-0.227	
18.12						
H(0)	2.840e-28					
H2	1.420e-28	1.657e-28	-27.848	-27.781	0.067	
28.57						
Mg	4.800e-02					
Mg+2	4.234e-02	1.009e-02	-1.373	-1.996	-0.623	-
22.42						

MgSO4	4.502e-03	5.252e-03	-2.347	-2.280	0.067	
7.11						
MgOH+	1.045e-03	7.057e-04	-2.981	-3.151	-0.170	
(0)						
MgHCO3+	6.461e-05	3.835e-05	-4.190	-4.416	-0.227	
6.29						
MgCO3	4.550e-05	5.309e-05	-4.342	-4.275	0.067	-
17.08						
Na	4.450e-01					
Na+	4.429e-01	2.999e-01	-0.354	-0.523	-0.169	
1.02						
NaSO4-	1.839e-03	1.184e-03	-2.735	-2.927	-0.191	
16.80						
NaCO3-	2.342e-04	1.674e-04	-3.630	-3.776	-0.146	
3.76						
NaHCO3	1.869e-05	2.181e-05	-4.728	-4.661	0.067	
1.80						
NaOH	1.574e-15	1.836e-15	-14.803	-14.736	0.067	
(0)						
O(0)	4.184e-20					
O2	2.092e-20	2.441e-20	-19.679	-19.612	0.067	
33.54						
S(6)	1.100e-02					
MgSO4	4.502e-03	5.252e-03	-2.347	-2.280	0.067	
7.11						
SO4-2	3.774e-03	5.615e-04	-2.423	-3.251	-0.827	
19.66						
NaSO4-	1.839e-03	1.184e-03	-2.735	-2.927	-0.191	
16.80						
CaSO4	8.846e-04	1.032e-03	-3.053	-2.986	0.067	
8.76						
HSO4-	2.639e-09	1.886e-09	-8.579	-8.724	-0.146	
42.34						
CaHSO4+	2.198e-10	1.571e-10	-9.658	-9.804	-0.146	
(0)						

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

Phase	SI**	log IAP	log K(363 K,	1 atm)
Anhydrite	-0.29	-5.41	-5.12	CaSO4
Aragonite	1.16	-7.85	-9.02	CaCO3
Calcite	1.27	-7.85	-9.12	CaCO3
CO2(g)	-3.63	-5.57	-1.94	CO2
Dolomite	2.79	-15.54	-18.33	CaMg(CO3)2
Gypsum	-0.64	-5.43	-4.79	CaSO4:2H2O
H2(g)	-24.66	-27.78	-3.12	H2
H2O(g)	-0.17	-0.01	0.16	H2O
Halite	-2.61	-0.99	1.61	NaCl
O2(g)	-16.50	-19.61	-3.11	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.

Using pressure 1.

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

Elements	Molality	Moles
C	8.224e-04	8.224e-04
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

	pH =	8.199	Charge balance
	pe =	-3.039	Adjusted to redox
equilibrium			
Specific Conductance ($\mu\text{S}/\text{cm}$, 90°C)	=	125758	
Density (g/cm^3)	=	0.98976	
Volume (L)	=	1.04491	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.694e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	2.400e-03	
Total CO2 (mol/kg)	=	8.224e-04	
Temperature (°C)	=	90.00	
Pressure (atm)	=	10.89	
Electrical balance (eq)	=	1.460e-02	
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.24	
Iterations	=	11	
Total H	=	1.110140e+02	
Total O	=	5.555383e+01	

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

mole V Species cm^3/mol	Molality	Activity	Log		Log	
			Molality	Activity	Gamma	
OH-	1.076e-04	6.157e-05	-3.968	-4.211	-0.242	-
3.11 H+	8.654e-09	6.320e-09	-8.063	-8.199	-0.137	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.65 C(-4)	4.280e-31					

CH4	4.280e-31	4.993e-31	-30.369	-30.302	0.067	
40.21						
C(4)	8.224e-04					
HCO3-	2.706e-04	1.742e-04	-3.568	-3.759	-0.191	
27.62						
NaCO3-	2.348e-04	1.679e-04	-3.629	-3.775	-0.146	
3.84						
CaCO3	1.368e-04	1.596e-04	-3.864	-3.797	0.067	-
14.39						
MgHCO3+	6.440e-05	3.824e-05	-4.191	-4.418	-0.226	
6.32						
MgCO3	4.564e-05	5.325e-05	-4.341	-4.274	0.067	-
17.01						
CaHCO3+	3.720e-05	2.462e-05	-4.429	-4.609	-0.179	
11.10						
NaHCO3	1.879e-05	2.193e-05	-4.726	-4.659	0.067	
1.80						
CO3-2	1.188e-05	2.044e-06	-4.925	-5.690	-0.765	-
7.25						
CO2	2.275e-06	2.654e-06	-5.643	-5.576	0.067	
38.08						
(CO2)2	4.897e-13	5.713e-13	-12.310	-12.243	0.067	
76.16						
Ca	3.500e-02					
Ca+2	3.394e-02	6.934e-03	-1.469	-2.159	-0.690	-
16.77						
CaSO4	8.848e-04	1.032e-03	-3.053	-2.986	0.067	
8.78						
CaCO3	1.368e-04	1.596e-04	-3.864	-3.797	0.067	-
14.39						
CaHCO3+	3.720e-05	2.462e-05	-4.429	-4.609	-0.179	
11.10						
CaOH+	2.500e-07	1.788e-07	-6.602	-6.748	-0.146	
(0)						
CaHSO4+	2.208e-10	1.578e-10	-9.656	-9.802	-0.146	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.395e-01	-0.243	-0.469	-0.227	
18.12						
H(0)	3.370e-14					
H2	1.685e-14	1.966e-14	-13.773	-13.706	0.067	
28.57						
Mg	4.800e-02					
Mg+2	4.235e-02	1.011e-02	-1.373	-1.995	-0.622	-
22.34						
MgSO4	4.497e-03	5.247e-03	-2.347	-2.280	0.067	
7.13						
MgOH+	1.043e-03	7.045e-04	-2.982	-3.152	-0.170	
(0)						
MgHCO3+	6.440e-05	3.824e-05	-4.191	-4.418	-0.226	
6.32						
MgCO3	4.564e-05	5.325e-05	-4.341	-4.274	0.067	-
17.01						
Na	4.450e-01					
Na+	4.429e-01	3.000e-01	-0.354	-0.523	-0.169	
1.05						

NaSO4-	1.844e-03	1.187e-03	-2.734	-2.925	-0.191
16.76					
NaCO3-	2.348e-04	1.679e-04	-3.629	-3.775	-0.146
3.84					
NaHCO3	1.879e-05	2.193e-05	-4.726	-4.659	0.067
1.80					
NaOH	1.582e-15	1.846e-15	-14.801	-14.734	0.067
(0)					
O(0)	0.000e+00				
O2	0.000e+00	0.000e+00	-47.836	-47.769	0.067
33.51					
S(-2)	1.968e-27				
HS-	1.943e-27	1.112e-27	-26.712	-26.954	-0.242
21.72					
H2S	2.003e-29	2.337e-29	-28.698	-28.631	0.067
37.28					
S-2	5.226e-30	8.279e-31	-29.282	-30.082	-0.800
(0)					
S(6)	1.100e-02				
MgSO4	4.497e-03	5.247e-03	-2.347	-2.280	0.067
7.13					
SO4-2	3.774e-03	5.621e-04	-2.423	-3.250	-0.827
19.66					
NaSO4-	1.844e-03	1.187e-03	-2.734	-2.925	-0.191
16.76					
CaSO4	8.848e-04	1.032e-03	-3.053	-2.986	0.067
8.78					
HSO4-	2.626e-09	1.877e-09	-8.581	-8.726	-0.146
42.31					
CaHSO4+	2.208e-10	1.578e-10	-9.656	-9.802	-0.146
(0)					

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

Phase	SI**	log IAP	log K(363 K, 11 atm)	
Anhydrite	-0.30	-5.41	-5.11	CaSO4
Aragonite	1.16	-7.85	-9.01	CaCO3
Calcite	1.26	-7.85	-9.11	CaCO3
CH4(g)	-27.28	-30.30	-3.02	CH4
CO2(g)	-3.63	-5.58	-1.95	CO2
Dolomite	2.78	-15.53	-18.31	CaMg(CO3)2
Gypsum	-0.64	-5.43	-4.79	CaSO4:2H2O
H2(g)	-10.59	-13.71	-3.12	H2
H2O(g)	-0.17	-0.01	0.16	H2O
H2S(g)	-27.21	-35.15	-7.94	H2S
Halite	-2.61	-0.99	1.61	NaCl
O2(g)	-44.65	-47.77	-3.12	O2
Sulfur	-21.94	-18.31	3.63	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.144 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=100.pqi

Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 10.89 atm, T variable\T=100.pqi

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 100
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
10.89

Beginning of initial solution calculations.

Initial solution 1.

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

--

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

--

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 100°C)	=	137325
Density (g/cm^3)	=	0.98245
Volume (L)	=	1.05266
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.680e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	2.839e-04
Total CO2 (mol/kg)	=	2.839e-04
Temperature ($^\circ\text{C}$)	=	100.00
Electrical balance (eq)	=	1.460e-02
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.24
Iterations	=	8
Total H	=	1.110145e+02
Total O	=	5.555302e+01

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	1.590e-04	8.984e-05	-3.799	-4.047	-0.248	-
3.59						
H+	8.698e-09	6.310e-09	-8.061	-8.200	-0.139	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.80						
C(4)	2.839e-04					
NaCO3-	9.379e-05	6.646e-05	-4.028	-4.177	-0.150	
3.04						
HCO3-	8.284e-05	5.283e-05	-4.082	-4.277	-0.195	
27.27						
CaCO3	4.958e-05	5.783e-05	-4.305	-4.238	0.067	-
14.43						
MgHCO3+	2.135e-05	1.253e-05	-4.671	-4.902	-0.231	
6.19						

MgCO3	1.443e-05	1.683e-05	-4.841	-4.774	0.067	-
17.07						
CaHCO3+	1.222e-05	8.013e-06	-4.913	-5.096	-0.183	
11.12						
NaHCO3	5.383e-06	6.278e-06	-5.269	-5.202	0.067	
1.80						
CO3-2	3.541e-06	5.857e-07	-5.451	-6.232	-0.781	-
9.60						
CO2	7.779e-07	9.073e-07	-6.109	-6.042	0.067	
38.89						
(CO2) 2	6.551e-14	7.640e-14	-13.184	-13.117	0.067	
77.78						
Ca	3.500e-02					
Ca+2	3.410e-02	6.684e-03	-1.467	-2.175	-0.708	-
17.07						
CaSO4	8.387e-04	9.782e-04	-3.076	-3.010	0.067	
8.86						
CaCO3	4.958e-05	5.783e-05	-4.305	-4.238	0.067	-
14.43						
CaHCO3+	1.222e-05	8.013e-06	-4.913	-5.096	-0.183	
11.12						
CaOH+	2.435e-07	1.725e-07	-6.614	-6.763	-0.150	
(0)						
CaHSO4+	2.692e-10	1.908e-10	-9.570	-9.719	-0.150	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.353e-01	-0.243	-0.475	-0.232	
17.63						
H(0)	2.661e-28					
H2	1.331e-28	1.552e-28	-27.876	-27.809	0.067	
28.57						
Mg	4.800e-02					
Mg+2	4.147e-02	9.516e-03	-1.382	-2.022	-0.639	-
22.83						
MgSO4	4.701e-03	5.482e-03	-2.328	-2.261	0.067	
7.20						
MgOH+	1.796e-03	1.203e-03	-2.746	-2.920	-0.174	
(0)						
MgHCO3+	2.135e-05	1.253e-05	-4.671	-4.902	-0.231	
6.19						
MgCO3	1.443e-05	1.683e-05	-4.841	-4.774	0.067	-
17.07						
Na	4.450e-01					
Na+	4.431e-01	2.966e-01	-0.353	-0.528	-0.174	
1.15						
NaSO4-	1.790e-03	1.141e-03	-2.747	-2.943	-0.195	
15.36						
NaCO3-	9.379e-05	6.646e-05	-4.028	-4.177	-0.150	
3.04						
NaHCO3	5.383e-06	6.278e-06	-5.269	-5.202	0.067	
1.80						
NaOH	2.285e-15	2.665e-15	-14.641	-14.574	0.067	
(0)						
O(0)	6.245e-18					
O2	3.122e-18	3.642e-18	-17.506	-17.439	0.067	
33.90						
S(6)	1.100e-02					

MgSO4	4.701e-03	5.482e-03	-2.328	-2.261	0.067
7.20					
SO4-2	3.671e-03	5.250e-04	-2.435	-3.280	-0.845
19.08					
NaSO4-	1.790e-03	1.141e-03	-2.747	-2.943	-0.195
15.36					
CaSO4	8.387e-04	9.782e-04	-3.076	-3.010	0.067
8.86					
HSO4-	3.350e-09	2.374e-09	-8.475	-8.625	-0.150
42.18					
CaHSO4+	2.692e-10	1.908e-10	-9.570	-9.719	-0.150
(0)					

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

--

Phase	SI**	log IAP	log K(373 K,	1 atm)
Anhydrite	-0.19	-5.45	-5.26	CaSO4
Aragonite	0.76	-8.41	-9.17	CaCO3
Calcite	0.86	-8.41	-9.27	CaCO3
CO2 (g)	-4.06	-6.04	-1.98	CO2
Dolomite	1.82	-16.66	-18.48	CaMg (CO3) 2
Gypsum	-0.62	-5.47	-4.85	CaSO4:2H2O
H2 (g)	-24.71	-27.81	-3.10	H2
H2O (g)	-0.01	-0.01	0.00	H2O
Halite	-2.62	-1.00	1.62	NaCl
O2 (g)	-14.32	-17.44	-3.11	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.

Using pressure 1.

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

--

Elements	Molality	Moles
C	2.839e-04	2.839e-04
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

pH = 8.200 Charge balance

```

pe = -2.920 Adjusted to redox
equilibrium
  Specific Conductance (µS/cm, 100°C) = 137231
    Density (g/cm³) = 0.98291
      Volume (L) = 1.05217
        Activity of water = 0.981
          Ionic strength (mol/kgw) = 6.680e-01
            Mass of water (kg) = 1.000e+00
              Total alkalinity (eq/kg) = 2.400e-03
                Total CO2 (mol/kg) = 2.839e-04
                  Temperature (°C) = 100.00
                    Pressure (atm) = 10.89
                      Electrical balance (eq) = 1.460e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.24
Iterations = 12
Total H = 1.110145e+02
Total O = 5.555302e+01

```

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

mole V Species cm³/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	1.599e-04	9.043e-05	-3.796	-4.044	-0.248	-
3.64 H+	8.702e-09	6.314e-09	-8.060	-8.200	-0.139	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.79 C(-4)	1.416e-33					
CH4	1.416e-33	1.652e-33	-32.849	-32.782	0.067	
41.05 C(4)	2.839e-04					
NaCO3-	9.407e-05	6.667e-05	-4.027	-4.176	-0.150	
3.13 HCO3-	8.243e-05	5.259e-05	-4.084	-4.279	-0.195	
27.29 CaCO3	4.978e-05	5.805e-05	-4.303	-4.236	0.067	-
14.37 MgHCO3+	2.126e-05	1.248e-05	-4.672	-4.904	-0.231	
6.22 MgCO3	1.447e-05	1.688e-05	-4.839	-4.773	0.067	-
17.00 CaHCO3+	1.217e-05	7.983e-06	-4.915	-5.098	-0.183	
11.14 NaHCO3	5.406e-06	6.305e-06	-5.267	-5.200	0.067	
1.80 CO3-2	3.560e-06	5.895e-07	-5.449	-6.229	-0.781	-
9.47 CO2	7.673e-07	8.948e-07	-6.115	-6.048	0.067	
38.86 (CO2)2	6.372e-14	7.432e-14	-13.196	-13.129	0.067	
77.73 Ca	3.500e-02					

Ca+2	3.410e-02	6.693e-03	-1.467	-2.174	-0.707	-
17.01						
CaSO4	8.389e-04	9.784e-04	-3.076	-3.009	0.067	
8.88						
CaCO3	4.978e-05	5.805e-05	-4.303	-4.236	0.067	-
14.37						
CaHCO3+	1.217e-05	7.983e-06	-4.915	-5.098	-0.183	
11.14						
CaOH+	2.437e-07	1.727e-07	-6.613	-6.763	-0.150	
(0)						
CaHSO4+	2.702e-10	1.915e-10	-9.568	-9.718	-0.150	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.354e-01	-0.243	-0.474	-0.232	
17.63						
H(0)	1.823e-14					
H2	9.114e-15	1.063e-14	-14.040	-13.973	0.067	
28.56						
Mg	4.800e-02					
Mg+2	4.147e-02	9.529e-03	-1.382	-2.021	-0.639	-
22.75						
MgSO4	4.696e-03	5.477e-03	-2.328	-2.261	0.067	
7.22						
MgOH+	1.795e-03	1.203e-03	-2.746	-2.920	-0.174	
(0)						
MgHCO3+	2.126e-05	1.248e-05	-4.672	-4.904	-0.231	
6.22						
MgCO3	1.447e-05	1.688e-05	-4.839	-4.773	0.067	-
17.00						
Na	4.450e-01					
Na+	4.431e-01	2.967e-01	-0.353	-0.528	-0.174	
1.18						
NaSO4-	1.795e-03	1.145e-03	-2.746	-2.941	-0.195	
15.33						
NaCO3-	9.407e-05	6.667e-05	-4.027	-4.176	-0.150	
3.13						
NaHCO3	5.406e-06	6.305e-06	-5.267	-5.200	0.067	
1.80						
NaOH	2.299e-15	2.681e-15	-14.638	-14.572	0.067	
(0)						
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-45.184	-45.118	0.067	
33.87						
S(-2)	2.216e-29					
HS-	2.184e-29	1.235e-29	-28.661	-28.908	-0.248	
21.41						
H2S	2.206e-31	2.573e-31	-30.656	-30.590	0.067	
37.29						
S-2	9.470e-32	1.442e-32	-31.024	-31.841	-0.817	
(0)						
S(6)	1.100e-02					
MgSO4	4.696e-03	5.477e-03	-2.328	-2.261	0.067	
7.22						
SO4-2	3.671e-03	5.256e-04	-2.435	-3.279	-0.844	
19.08						
NaSO4-	1.795e-03	1.145e-03	-2.746	-2.941	-0.195	
15.33						

CaSO4	8.389e-04	9.784e-04	-3.076	-3.009	0.067
8.88					
HSO4-	3.330e-09	2.360e-09	-8.478	-8.627	-0.150
42.16					
CaHSO4+	2.702e-10	1.915e-10	-9.568	-9.718	-0.150
(0)					

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

Phase	SI**	log IAP	log K(373 K, 11 atm)	
Anhydrite	-0.20	-5.45	-5.26	CaSO4
Aragonite	0.75	-8.40	-9.16	CaCO3
Calcite	0.85	-8.40	-9.26	CaCO3
CH4(g)	-29.77	-32.78	-3.01	CH4
CO2(g)	-4.06	-6.05	-1.98	CO2
Dolomite	1.81	-16.65	-18.46	CaMg(CO3)2
Gypsum	-0.63	-5.47	-4.84	CaSO4:2H2O
H2(g)	-10.87	-13.97	-3.10	H2
H2O(g)	-0.01	-0.01	0.00	H2O
H2S(g)	-29.16	-37.11	-7.95	H2S
Halite	-2.62	-1.00	1.62	NaCl
O2(g)	-42.00	-45.12	-3.12	O2
Sulfur	-23.51	-20.03	3.48	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.503 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=40.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=40.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
61.24

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67832
Density (g/cm^3)	=	1.01647
Volume (L)	=	1.01750
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.753e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.989e-03

Total CO2 (mol/kg) = 1.989e-03
 Temperature (°C) = 40.00
 Electrical balance (eq) = 1.460e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
 Iterations = 7
 Total H = 1.110141e+02
 Total O = 5.555622e+01

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

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm ³ /mol						
OH-	7.568e-06	4.553e-06	-5.121	-5.342	-0.221	-
2.19						
H+	8.413e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(4)	1.989e-03					
HCO3-	1.160e-03	7.764e-04	-2.935	-3.110	-0.174	
27.66						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
CO3-2	3.684e-05	7.386e-06	-4.434	-5.132	-0.698	-
1.66						
CO2	8.476e-06	9.902e-06	-5.072	-5.004	0.068	
35.16						
(CO2)2	2.427e-12	2.835e-12	-11.615	-11.547	0.068	
70.32						
Ca	3.500e-02					
Ca+2	3.360e-02	8.086e-03	-1.474	-2.092	-0.619	-
16.46						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
CaOH+	2.817e-07	2.087e-07	-6.550	-6.681	-0.130	
(0)						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						
Cl	5.720e-01					

Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	4.185e-28					
H2	2.093e-28	2.445e-28	-27.679	-27.612	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.244e-02	-1.350	-1.905	-0.555	-
20.81						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
MgOH+	3.650e-05	2.551e-05	-4.438	-4.593	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.142e-01	-0.354	-0.503	-0.149	
0.05						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
NaOH	1.225e-16	1.431e-16	-15.912	-15.844	0.068	
(0)						
O(0)	4.672e-33					
O2	2.336e-33	2.729e-33	-32.632	-32.564	0.068	
31.40						
S(6)	1.100e-02					
SO4-2	4.738e-03	8.290e-04	-2.324	-3.081	-0.757	
19.21						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
HSO4-	9.700e-10	7.187e-10	-9.013	-9.143	-0.130	
41.78						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.72	-5.17	-4.45	CaSO4
Aragonite	1.22	-7.22	-8.45	CaCO3
Calcite	1.36	-7.22	-8.58	CaCO3
CO2(g)	-3.38	-5.00	-1.63	CO2
Dolomite	3.16	-14.26	-17.42	CaMg(CO3)2
Gypsum	-0.59	-5.19	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O

Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-29.58	-32.56	-2.98	O2

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
C	1.989e-03	1.989e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

	pH =	8.178	Charge balance
	pe =	8.792	Adjusted to redox
equilibrium			
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67832	
Density (g/cm^3)	=	1.01901	
Volume (L)	=	1.01496	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.754e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	2.400e-03	
Total CO2 (mol/kg)	=	1.989e-03	
Temperature (°C)	=	40.00	
Pressure (atm)	=	61.24	
Electrical balance (eq)	=	1.460e-02	
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23	
Iterations	=	9	
Total H	=	1.110141e+02	
Total O	=	5.555622e+01	

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

			Log	Log	Log	
mole V	Species	Molality	Activity	Molality	Activity	Gamma
cm^3/mol						

OH-	7.535e-06	4.540e-06	-5.123	-5.343	-0.220	-
2.19						
H+	8.840e-09	6.636e-09	-8.054	-8.178	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.11						
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-118.452	-118.384	0.068	
36.68						
C(4)	1.989e-03					
HCO3-	1.152e-03	7.719e-04	-2.938	-3.112	-0.174	
27.71						
MgHCO3+	1.986e-04	1.237e-04	-3.702	-3.908	-0.206	
6.34						
CaHCO3+	1.382e-04	9.491e-05	-3.860	-4.023	-0.163	
10.57						
CaCO3	1.251e-04	1.462e-04	-3.903	-3.835	0.068	-
14.14						
NaCO3-	1.197e-04	8.880e-05	-3.922	-4.052	-0.130	
4.63						
NaHCO3	1.147e-04	1.339e-04	-3.941	-3.873	0.068	
1.80						
MgCO3	9.501e-05	1.110e-04	-4.022	-3.955	0.068	-
16.65						
CO3-2	3.708e-05	7.471e-06	-4.431	-5.127	-0.696	-
1.17						
CO2	8.349e-06	9.753e-06	-5.078	-5.011	0.068	
35.11						
(CO2)2	2.354e-12	2.750e-12	-11.628	-11.561	0.068	
70.22						
Ca	3.500e-02					
Ca+2	3.360e-02	8.127e-03	-1.474	-2.090	-0.616	-
16.06						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
8.12						
CaHCO3+	1.382e-04	9.491e-05	-3.860	-4.023	-0.163	
10.57						
CaCO3	1.251e-04	1.462e-04	-3.903	-3.835	0.068	-
14.14						
CaOH+	2.702e-07	2.004e-07	-6.568	-6.698	-0.130	
(0)						
CaHSO4+	1.010e-10	7.489e-11	-9.996	-10.126	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.571e-01	-0.243	-0.447	-0.205	
19.09						
H(0)	1.129e-37					
H2	5.645e-38	6.594e-38	-37.248	-37.181	0.068	
28.56						
Mg	4.800e-02					
Mg+2	4.470e-02	1.251e-02	-1.350	-1.903	-0.553	-
20.36						
MgSO4	2.972e-03	3.472e-03	-2.527	-2.459	0.068	
6.46						
MgHCO3+	1.986e-04	1.237e-04	-3.702	-3.908	-0.206	
6.34						

MgCO3	9.501e-05	1.110e-04	-4.022	-3.955	0.068	-
16.65						
MgOH+	3.467e-05	2.426e-05	-4.460	-4.615	-0.155	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.147e-01	-0.354	-0.502	-0.148	
0.23						
NaSO4-	2.145e-03	1.437e-03	-2.669	-2.843	-0.174	
20.50						
NaCO3-	1.197e-04	8.880e-05	-3.922	-4.052	-0.130	
4.63						
NaHCO3	1.147e-04	1.339e-04	-3.941	-3.873	0.068	
1.80						
NaOH	1.217e-16	1.422e-16	-15.915	-15.847	0.068	
(0)						
O(0)	5.682e-14					
O2	2.841e-14	3.319e-14	-13.547	-13.479	0.068	
31.28						
S(-2)	0.000e+00					
HS-	0.000e+00	0.000e+00	-115.302	-115.522	-0.220	
21.90						
H2S	0.000e+00	0.000e+00	-117.010	-116.943	0.068	
37.10						
S-2	0.000e+00	0.000e+00	-119.087	-119.815	-0.728	
(0)						
S(6)	1.100e-02					
SO4-2	4.748e-03	8.349e-04	-2.324	-3.078	-0.755	
18.96						
MgSO4	2.972e-03	3.472e-03	-2.527	-2.459	0.068	
6.46						
NaSO4-	2.145e-03	1.437e-03	-2.669	-2.843	-0.174	
20.50						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
8.12						
HSO4-	9.734e-10	7.219e-10	-9.012	-9.142	-0.130	
41.61						
CaHSO4+	1.010e-10	7.489e-11	-9.996	-10.126	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	61 atm)
Anhydrite	-0.76	-5.17	-4.41	CaSO4
Aragonite	1.18	-7.22	-8.39	CaCO3
Calcite	1.31	-7.22	-8.52	CaCO3
CH4(g)	-115.43	-118.38	-2.95	CH4
CO2(g)	-3.35	-5.01	-1.66	CO2
Dolomite	3.07	-14.25	-17.32	CaMg(CO3)2
Gypsum	-0.62	-5.18	-4.56	CaSO4:2H2O
H2(g)	-34.02	-37.18	-3.16	H2
H2O(g)	-1.13	-0.01	1.12	H2O
H2S(g)	-115.72	-123.70	-7.98	H2S
Halite	-2.54	-0.95	1.59	NaCl
O2(g)	-10.46	-13.48	-3.02	O2
Sulfur	-87.51	-83.00	4.51	S

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.487 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=42.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=42.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 42
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg

REACTION_PRESSURE 1
61.24

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 42°C)	=	70069
Density (g/cm^3)	=	1.01565
Volume (L)	=	1.01832
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.751e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.963e-03
Total CO2 (mol/kg)	=	1.963e-03
Temperature (°C)	=	42.00
Electrical balance (eq)	=	1.460e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23
Iterations	=	7
Total H	=	1.110140e+02
Total O	=	5.555615e+01

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

mole V Species cm^3/mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	8.634e-06	5.186e-06	-5.064	-5.285	-0.221	-
2.17 H+	8.420e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.17 C(4)	1.963e-03					
HCO3-	1.127e-03	7.534e-04	-2.948	-3.123	-0.175	
27.71						

MgHCO3+	1.945e-04	1.208e-04	-3.711	-3.918	-0.207	
6.19						
CaHCO3+	1.355e-04	9.285e-05	-3.868	-4.032	-0.164	
10.49						
NaCO3-	1.306e-04	9.662e-05	-3.884	-4.015	-0.131	
4.21						
CaCO3	1.299e-04	1.517e-04	-3.886	-3.819	0.068	-
14.55						
NaHCO3	1.039e-04	1.214e-04	-3.983	-3.916	0.068	
1.80						
MgCO3	9.631e-05	1.125e-04	-4.016	-3.949	0.068	-
17.10						
CO3-2	3.684e-05	7.349e-06	-4.434	-5.134	-0.700	-
1.70						
CO2	8.154e-06	9.526e-06	-5.089	-5.021	0.068	
35.26						
(CO2) 2	2.372e-12	2.771e-12	-11.625	-11.557	0.068	
70.52						
Ca	3.500e-02					
Ca+2	3.361e-02	8.043e-03	-1.474	-2.095	-0.621	-
16.44						
CaSO4	1.127e-03	1.316e-03	-2.948	-2.881	0.068	
8.01						
CaHCO3+	1.355e-04	9.285e-05	-3.868	-4.032	-0.164	
10.49						
CaCO3	1.299e-04	1.517e-04	-3.886	-3.819	0.068	-
14.55						
CaOH+	2.805e-07	2.076e-07	-6.552	-6.683	-0.131	
(0)						
CaHSO4+	9.702e-11	7.180e-11	-10.013	-10.144	-0.131	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.560e-01	-0.243	-0.449	-0.206	
19.09						
H(0)	4.111e-28					
H2	2.056e-28	2.401e-28	-27.687	-27.620	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.461e-02	1.236e-02	-1.351	-1.908	-0.557	-
20.86						
MgSO4	3.061e-03	3.576e-03	-2.514	-2.447	0.068	
6.35						
MgHCO3+	1.945e-04	1.208e-04	-3.711	-3.918	-0.207	
6.19						
MgCO3	9.631e-05	1.125e-04	-4.016	-3.949	0.068	-
17.10						
MgOH+	4.271e-05	2.981e-05	-4.369	-4.526	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.138e-01	-0.354	-0.503	-0.149	
0.11						
NaSO4-	2.125e-03	1.420e-03	-2.673	-2.848	-0.175	
20.82						
NaCO3-	1.306e-04	9.662e-05	-3.884	-4.015	-0.131	
4.21						
NaHCO3	1.039e-04	1.214e-04	-3.983	-3.916	0.068	
1.80						

NaOH	1.393e-16	1.627e-16	-15.856	-15.789	0.068
(0)					
O(0)	1.847e-32				
O2	9.236e-33	1.079e-32	-32.035	-31.967	0.068
31.51					
S(6)	1.100e-02				
SO4-2	4.687e-03	8.157e-04	-2.329	-3.088	-0.759
19.36					
MgSO4	3.061e-03	3.576e-03	-2.514	-2.447	0.068
6.35					
NaSO4-	2.125e-03	1.420e-03	-2.673	-2.848	-0.175
20.82					
CaSO4	1.127e-03	1.316e-03	-2.948	-2.881	0.068
8.01					
HSO4-	1.003e-09	7.425e-10	-8.999	-9.129	-0.131
41.86					
CaHSO4+	9.702e-11	7.180e-11	-10.013	-10.144	-0.131
(0)					

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

Phase	SI**	log IAP	log K(315 K,	1 atm)
Anhydrite	-0.71	-5.18	-4.48	CaSO4
Aragonite	1.23	-7.23	-8.46	CaCO3
Calcite	1.37	-7.23	-8.60	CaCO3
CO2(g)	-3.38	-5.02	-1.64	CO2
Dolomite	3.19	-14.27	-17.46	CaMg(CO3)2
Gypsum	-0.60	-5.20	-4.60	CaSO4:2H2O
H2(g)	-24.49	-27.62	-3.13	H2
H2O(g)	-1.10	-0.01	1.09	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-28.97	-31.97	-2.99	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
C	1.963e-03	1.963e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01

S 1.100e-02 1.100e-02

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

pH = 8.178 Charge balance
 pe = 8.379 Adjusted to redox
 equilibrium
 Specific Conductance ($\mu\text{S}/\text{cm}$, 42°C) = 70054
 Density (g/cm^3) = 1.01818
 Volume (L) = 1.01578
 Activity of water = 0.981
 Ionic strength (mol/kgw) = 6.751e-01
 Mass of water (kg) = 1.000e+00
 Total alkalinity (eq/kg) = 2.400e-03
 Total CO2 (mol/kg) = 1.963e-03
 Temperature (°C) = 42.00
 Pressure (atm) = 61.24
 Electrical balance (eq) = 1.460e-02
 Percent error, $100 * (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = 1.23
 Iterations = 10
 Total H = 1.110140e+02
 Total O = 5.555615e+01

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

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH- 2.18	8.601e-06	5.174e-06	-5.065	-5.286	-0.221	-
H+ 0.00	8.840e-09	6.630e-09	-8.054	-8.178	-0.125	
H2O 18.12	5.551e+01	9.812e-01	1.744	-0.008	0.000	
C(-4) CH4 36.82	0.000e+00	0.000e+00	-115.426	-115.358	0.068	
C(4) HCO3- 27.77	1.963e-03	7.489e-04	-2.951	-3.126	-0.174	
MgHCO3+ 6.37	1.119e-03	1.210e-04	-3.711	-3.917	-0.206	
CaHCO3+ 10.61	1.945e-04	9.302e-05	-3.868	-4.031	-0.164	
CaCO3 14.14	1.356e-04	1.532e-04	-3.882	-3.815	0.068	-
NaCO3- 4.73	1.312e-04	9.665e-05	-3.884	-4.015	-0.130	
NaHCO3 1.80	1.305e-04	1.284e-04	-3.959	-3.891	0.068	
MgCO3 16.66	1.099e-04	1.132e-04	-4.014	-3.946	0.068	-

CO3-2	3.710e-05	7.438e-06	-4.431	-5.129	-0.698	-
1.22						
CO2	8.025e-06	9.375e-06	-5.096	-5.028	0.068	
35.20						
(CO2)2	2.298e-12	2.684e-12	-11.639	-11.571	0.068	
70.41						
Ca	3.500e-02					
Ca+2	3.361e-02	8.084e-03	-1.474	-2.092	-0.619	-
16.04						
CaSO4	1.127e-03	1.316e-03	-2.948	-2.881	0.068	
8.16						
CaHCO3+	1.356e-04	9.302e-05	-3.868	-4.031	-0.164	
10.61						
CaCO3	1.312e-04	1.532e-04	-3.882	-3.815	0.068	-
14.14						
CaOH+	2.694e-07	1.995e-07	-6.570	-6.700	-0.130	
(0)						
CaHSO4+	1.038e-10	7.690e-11	-9.984	-10.114	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.565e-01	-0.243	-0.448	-0.205	
19.10						
H(0)	7.407e-37					
H2	3.703e-37	4.326e-37	-36.431	-36.364	0.068	
28.56						
Mg	4.800e-02					
Mg+2	4.463e-02	1.242e-02	-1.350	-1.906	-0.555	-
20.41						
MgSO4	3.043e-03	3.554e-03	-2.517	-2.449	0.068	
6.50						
MgHCO3+	1.945e-04	1.210e-04	-3.711	-3.917	-0.206	
6.37						
MgCO3	9.687e-05	1.132e-04	-4.014	-3.946	0.068	-
16.66						
MgOH+	4.060e-05	2.837e-05	-4.391	-4.547	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.142e-01	-0.354	-0.503	-0.149	
0.29						
NaSO4-	2.135e-03	1.429e-03	-2.671	-2.845	-0.174	
20.43						
NaCO3-	1.305e-04	9.665e-05	-3.884	-4.015	-0.130	
4.73						
NaHCO3	1.099e-04	1.284e-04	-3.959	-3.891	0.068	
1.80						
NaOH	1.386e-16	1.619e-16	-15.858	-15.791	0.068	
(0)						
O(0)	5.038e-15					
O2	2.519e-15	2.943e-15	-14.599	-14.531	0.068	
31.39						
S(-2)	0.000e+00					
HS-	0.000e+00	0.000e+00	-112.276	-112.497	-0.221	
21.94						
H2S	0.000e+00	0.000e+00	-114.004	-113.937	0.068	
37.11						
S-2	0.000e+00	0.000e+00	-116.006	-116.736	-0.730	
(0)						

S (6)	1.100e-02					
SO4-2	4.695e-03	8.213e-04	-2.328	-3.086	-0.757	
19.12						
MgSO4	3.043e-03	3.554e-03	-2.517	-2.449	0.068	
6.50						
NaSO4-	2.135e-03	1.429e-03	-2.671	-2.845	-0.174	
20.43						
CaSO4	1.127e-03	1.316e-03	-2.948	-2.881	0.068	
8.16						
HSO4-	1.006e-09	7.453e-10	-8.997	-9.128	-0.130	
41.69						
CaHSO4+	1.038e-10	7.690e-11	-9.984	-10.114	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(315 K, 61 atm)	
Anhydrite	-0.75	-5.18	-4.43	CaSO4
Aragonite	1.19	-7.22	-8.41	CaCO3
Calcite	1.32	-7.22	-8.54	CaCO3
CH4 (g)	-112.40	-115.36	-2.96	CH4
CO2 (g)	-3.35	-5.03	-1.68	CO2
Dolomite	3.10	-14.26	-17.36	CaMg (CO3) 2
Gypsum	-0.63	-5.19	-4.57	CaSO4:2H2O
H2 (g)	-33.21	-36.36	-3.16	H2
H2O (g)	-1.08	-0.01	1.07	H2O
H2S (g)	-112.69	-120.68	-7.98	H2S
Halite	-2.54	-0.95	1.59	NaCl
O2 (g)	-11.50	-14.53	-3.03	O2
Sulfur	-85.29	-80.82	4.47	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.153 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=45.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=45.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 45
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
61.24

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH = 8.200
pe = 4.000

Specific Conductance ($\mu\text{S}/\text{cm}$, 45°C) = 73449
 Density (g/cm^3) = 1.01436
 Volume (L) = 1.01961
 Activity of water = 0.981
 Ionic strength (mol/kgw) = $6.747\text{e-}01$
 Mass of water (kg) = $1.000\text{e+}00$
 Total carbon (mol/kg) = $1.922\text{e-}03$
 Total CO_2 (mol/kg) = $1.922\text{e-}03$
 Temperature ($^\circ\text{C}$) = 45.00
 Electrical balance (eq) = $1.460\text{e-}02$
 Percent error, $100 * (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = 1.23
 Iterations = 7
 Total H = $1.110140\text{e+}02$
 Total O = $5.555604\text{e+}01$

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	$1.047\text{e-}05$	$6.273\text{e-}06$	-4.980	-5.202	-0.222	-
2.14						
H+	$8.431\text{e-}09$	$6.310\text{e-}09$	-8.074	-8.200	-0.126	
0.00						
H ₂ O	$5.551\text{e+}01$	$9.812\text{e-}01$	1.744	-0.008	0.000	
18.19						
C(4)	$1.922\text{e-}03$					
HCO ₃ -	$1.077\text{e-}03$	$7.181\text{e-}04$	-2.968	-3.144	-0.176	
27.79						
MgHCO ₃ +	$1.883\text{e-}04$	$1.166\text{e-}04$	-3.725	-3.933	-0.208	
6.23						
NaCO ₃ -	$1.472\text{e-}04$	$1.088\text{e-}04$	-3.832	-3.964	-0.132	
4.34						
CaCO ₃	$1.388\text{e-}04$	$1.621\text{e-}04$	-3.858	-3.790	0.067	-
14.55						
CaHCO ₃ +	$1.310\text{e-}04$	$8.963\text{e-}05$	-3.883	-4.048	-0.165	
10.56						
MgCO ₃	$9.848\text{e-}05$	$1.150\text{e-}04$	-4.007	-3.939	0.067	-
17.10						
NaHCO ₃	$9.732\text{e-}05$	$1.137\text{e-}04$	-4.012	-3.944	0.067	
1.80						
CO ₃ -2	$3.663\text{e-}05$	$7.250\text{e-}06$	-4.436	-5.140	-0.704	-
1.80						
CO ₂	$7.698\text{e-}06$	$8.992\text{e-}06$	-5.114	-5.046	0.067	
35.41						
(CO ₂) ₂	$2.289\text{e-}12$	$2.674\text{e-}12$	-11.640	-11.573	0.067	
70.81						
Ca	$3.500\text{e-}02$					
Ca+2	$3.362\text{e-}02$	$7.978\text{e-}03$	-1.473	-2.098	-0.625	-
16.43						
CaSO ₄	$1.113\text{e-}03$	$1.300\text{e-}03$	-2.954	-2.886	0.067	
8.08						
CaCO ₃	$1.388\text{e-}04$	$1.621\text{e-}04$	-3.858	-3.790	0.067	-
14.55						

CaHCO3+	1.310e-04	8.963e-05	-3.883	-4.048	-0.165	
10.56						
CaOH+	2.788e-07	2.059e-07	-6.555	-6.686	-0.132	
(0)						
CaHSO4+	1.013e-10	7.486e-11	-9.994	-10.126	-0.132	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.551e-01	-0.243	-0.450	-0.207	
19.10						
H(0)	4.004e-28					
H2	2.002e-28	2.339e-28	-27.699	-27.631	0.067	
28.59						
Mg	4.800e-02					
Mg+2	4.449e-02	1.223e-02	-1.352	-1.913	-0.561	-
20.95						
MgSO4	3.166e-03	3.698e-03	-2.499	-2.432	0.067	
6.42						
MgHCO3+	1.883e-04	1.166e-04	-3.725	-3.933	-0.208	
6.23						
MgCO3	9.848e-05	1.150e-04	-4.007	-3.939	0.067	-
17.10						
MgOH+	5.383e-05	3.751e-05	-4.269	-4.426	-0.157	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.130e-01	-0.354	-0.504	-0.151	
0.19						
NaSO4-	2.109e-03	1.406e-03	-2.676	-2.852	-0.176	
20.69						
NaCO3-	1.472e-04	1.088e-04	-3.832	-3.964	-0.132	
4.34						
NaHCO3	9.732e-05	1.137e-04	-4.012	-3.944	0.067	
1.80						
NaOH	1.681e-16	1.964e-16	-15.774	-15.707	0.067	
(0)						
O(0)	1.406e-31					
O2	7.029e-32	8.210e-32	-31.153	-31.086	0.067	
31.67						
S(6)	1.100e-02					
SO4-2	4.612e-03	7.961e-04	-2.336	-3.099	-0.763	
19.56						
MgSO4	3.166e-03	3.698e-03	-2.499	-2.432	0.067	
6.42						
NaSO4-	2.109e-03	1.406e-03	-2.676	-2.852	-0.176	
20.69						
CaSO4	1.113e-03	1.300e-03	-2.954	-2.886	0.067	
8.08						
HSO4-	1.056e-09	7.804e-10	-8.976	-9.108	-0.132	
41.96						
CaHSO4+	1.013e-10	7.486e-11	-9.994	-10.126	-0.132	
(0)						

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

Phase	SI**	log IAP	log K(318 K,	1 atm)
Anhydrite	-0.68	-5.20	-4.51	CaSO4

Aragonite	1.25	-7.24	-8.49	CaCO3
Calcite	1.38	-7.24	-8.62	CaCO3
CO2(g)	-3.38	-5.05	-1.67	CO2
Dolomite	3.23	-14.29	-17.52	CaMg(CO3)2
Gypsum	-0.61	-5.21	-4.61	CaSO4:2H2O
H2(g)	-24.50	-27.63	-3.13	H2
H2O(g)	-1.03	-0.01	1.03	H2O
Halite	-2.54	-0.95	1.59	NaCl
O2(g)	-28.08	-31.09	-3.01	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.

Using pressure 1.

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

--

Elements	Molality	Moles
C	1.922e-03	1.922e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	8.179	Charge balance
	pe =	8.224	Adjusted to redox
equilibrium			
	Specific Conductance (µS/cm, 45°C)	= 73412	
	Density (g/cm³)	= 1.01690	
	Volume (L)	= 1.01707	
	Activity of water	= 0.981	
	Ionic strength (mol/kgw)	= 6.747e-01	
	Mass of water (kg)	= 1.000e+00	
	Total alkalinity (eq/kg)	= 2.400e-03	
	Total CO2 (mol/kg)	= 1.922e-03	
	Temperature (°C)	= 45.00	
	Pressure (atm)	= 61.24	
	Electrical balance (eq)	= 1.460e-02	
Percent error, 100*(Cat- An)/(Cat+ An)		= 1.23	
	Iterations	= 10	
	Total H	= 1.110140e+02	
	Total O	= 5.555604e+01	

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

--

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.044e-05	6.267e-06	-4.981	-5.203	-0.222	-
2.18						
H+	8.838e-09	6.620e-09	-8.054	-8.179	-0.126	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.15						
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-114.591	-114.524	0.067	
37.03						
C(4)	1.922e-03					
HCO3-	1.069e-03	7.136e-04	-2.971	-3.147	-0.175	
27.84						
MgHCO3+	1.882e-04	1.168e-04	-3.725	-3.933	-0.207	
6.41						
NaCO3-	1.473e-04	1.089e-04	-3.832	-3.963	-0.131	
4.85						
CaCO3	1.403e-04	1.639e-04	-3.853	-3.786	0.067	-
14.14						
CaHCO3+	1.311e-04	8.978e-05	-3.882	-4.047	-0.164	
10.68						
NaHCO3	1.029e-04	1.202e-04	-3.987	-3.920	0.067	
1.80						
MgCO3	9.913e-05	1.158e-04	-4.004	-3.936	0.067	-
16.66						
CO3-2	3.693e-05	7.346e-06	-4.433	-5.134	-0.701	-
1.31						
CO2	7.565e-06	8.836e-06	-5.121	-5.054	0.067	
35.35						
(CO2)2	2.211e-12	2.583e-12	-11.655	-11.588	0.067	
70.70						
Ca	3.500e-02					
Ca+2	3.361e-02	8.020e-03	-1.473	-2.096	-0.622	-
16.03						
CaSO4	1.113e-03	1.301e-03	-2.953	-2.886	0.067	
8.23						
CaCO3	1.403e-04	1.639e-04	-3.853	-3.786	0.067	-
14.14						
CaHCO3+	1.311e-04	8.978e-05	-3.882	-4.047	-0.164	
10.68						
CaOH+	2.681e-07	1.982e-07	-6.572	-6.703	-0.131	
(0)						
CaHSO4+	1.083e-10	8.008e-11	-9.965	-10.096	-0.131	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.556e-01	-0.243	-0.449	-0.206	
19.11						
H(0)	1.474e-36					
H2	7.369e-37	8.607e-37	-36.133	-36.065	0.067	
28.56						

Mg	4.800e-02						
Mg+2	4.451e-02	1.230e-02	-1.352	-1.910	-0.559	-	
20.50							
MgSO4	3.148e-03	3.677e-03	-2.502	-2.435	0.067		
6.57							
MgHCO3+	1.882e-04	1.168e-04	-3.725	-3.933	-0.207		
6.41							
MgCO3	9.913e-05	1.158e-04	-4.004	-3.936	0.067	-	
16.66							
MgOH+	5.125e-05	3.576e-05	-4.290	-4.447	-0.156		
(0)							
Na	4.450e-01						
Na+	4.426e-01	3.135e-01	-0.354	-0.504	-0.150		
0.37							
NaSO4-	2.120e-03	1.416e-03	-2.674	-2.849	-0.175		
20.31							
NaCO3-	1.473e-04	1.089e-04	-3.832	-3.963	-0.131		
4.85							
NaHCO3	1.029e-04	1.202e-04	-3.987	-3.920	0.067		
1.80							
NaOH	1.675e-16	1.956e-16	-15.776	-15.709	0.067		
(0)							
O(0)	9.196e-15						
O2	4.598e-15	5.371e-15	-14.337	-14.270	0.067		
31.54							
S(-2)	0.000e+00						
HS-	0.000e+00	0.000e+00	-111.439	-111.661	-0.222		
22.00							
H2S	0.000e+00	0.000e+00	-113.195	-113.127	0.067		
37.12							
S-2	0.000e+00	0.000e+00	-115.086	-115.820	-0.734		
(0)							
S(6)	1.100e-02						
SO4-2	4.619e-03	8.014e-04	-2.335	-3.096	-0.761		
19.34							
MgSO4	3.148e-03	3.677e-03	-2.502	-2.435	0.067		
6.57							
NaSO4-	2.120e-03	1.416e-03	-2.674	-2.849	-0.175		
20.31							
CaSO4	1.113e-03	1.301e-03	-2.953	-2.886	0.067		
8.23							
HSO4-	1.058e-09	7.826e-10	-8.975	-9.106	-0.131		
41.79							
CaHSO4+	1.083e-10	8.008e-11	-9.965	-10.096	-0.131		
(0)							

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

Phase	SI**	log IAP	log K(318 K, 61 atm)	
Anhydrite	-0.72	-5.19	-4.47	CaSO4
Aragonite	1.21	-7.23	-8.44	CaCO3
Calcite	1.34	-7.23	-8.57	CaCO3
CH4 (g)	-111.55	-114.52	-2.97	CH4
CO2 (g)	-3.35	-5.05	-1.71	CO2
Dolomite	3.15	-14.27	-17.42	CaMg (CO3) 2

Gypsum	-0.64	-5.21	-4.57	CaSO4:2H2O
H2(g)	-32.90	-36.07	-3.16	H2
H2O(g)	-1.02	-0.01	1.01	H2O
H2S(g)	-111.86	-119.84	-7.98	H2S
Halite	-2.55	-0.95	1.59	NaCl
O2(g)	-11.23	-14.27	-3.04	O2
Sulfur	-84.73	-80.32	4.41	S

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.083 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=49.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=49.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 49
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1

```

Ca      35
Mg      48
Na     445
S(6)    11
Alkalinity 2.4 as HCO3-
Cl      572
water   1 # kg
REACTION PRESSURE 1
61.24

```

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

```

pH = 8.200
pe = 4.000
Specific Conductance (µS/cm, 49°C) = 77999
Density (g/cm³) = 1.01257
Volume (L) = 1.02142
Activity of water = 0.981
Ionic strength (mol/kgw) = 6.742e-01
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 1.864e-03
Total CO2 (mol/kg) = 1.864e-03
Temperature (°C) = 49.00
Electrical balance (eq) = 1.460e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
Iterations = 7
Total H = 1.110139e+02
Total O = 5.555589e+01

```

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

mole V Species cm ³ /mol	Molality	Activity	Log	Log	Log
			Molality	Activity	Gamma
OH- 2.12	1.343e-05	8.018e-06	-4.872	-5.096	-0.224

H+	8.447e-09	6.310e-09	-8.073	-8.200	-0.127	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.23						
C(4)	1.864e-03					
HCO3-	1.007e-03	6.700e-04	-2.997	-3.174	-0.177	
27.86						
MgHCO3+	1.796e-04	1.109e-04	-3.746	-3.955	-0.209	
6.28						
NaCO3-	1.702e-04	1.254e-04	-3.769	-3.902	-0.133	
4.47						
CaCO3	1.504e-04	1.757e-04	-3.823	-3.755	0.067	-
14.54						
CaHCO3+	1.242e-04	8.475e-05	-3.906	-4.072	-0.166	
10.64						
MgCO3	1.003e-04	1.171e-04	-3.999	-3.931	0.067	-
17.10						
NaHCO3	8.875e-05	1.037e-04	-4.052	-3.984	0.067	
1.80						
CO3-2	3.597e-05	7.042e-06	-4.444	-5.152	-0.708	-
1.99						
CO2	7.130e-06	8.327e-06	-5.147	-5.080	0.067	
35.61						
(CO2)2	2.174e-12	2.540e-12	-11.663	-11.595	0.067	
71.22						
Ca	3.500e-02					
Ca+2	3.363e-02	7.891e-03	-1.473	-2.103	-0.630	-
16.42						
CaSO4	1.094e-03	1.278e-03	-2.961	-2.894	0.067	
8.17						
CaCO3	1.504e-04	1.757e-04	-3.823	-3.755	0.067	-
14.54						
CaHCO3+	1.242e-04	8.475e-05	-3.906	-4.072	-0.166	
10.64						
CaOH+	2.764e-07	2.036e-07	-6.558	-6.691	-0.133	
(0)						
CaHSO4+	1.076e-10	7.927e-11	-9.968	-10.101	-0.133	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.539e-01	-0.243	-0.451	-0.209	
19.10						
H(0)	3.869e-28					
H2	1.934e-28	2.259e-28	-27.713	-27.646	0.067	
28.59						
Mg	4.800e-02					
Mg+2	4.434e-02	1.206e-02	-1.353	-1.919	-0.566	-
21.06						
MgSO4	3.305e-03	3.860e-03	-2.481	-2.413	0.067	
6.51						
MgHCO3+	1.796e-04	1.109e-04	-3.746	-3.955	-0.209	
6.28						
MgCO3	1.003e-04	1.171e-04	-3.999	-3.931	0.067	-
17.10						
MgOH+	7.277e-05	5.059e-05	-4.138	-4.296	-0.158	
(0)						
Na	4.450e-01					

Na+	4.427e-01	3.120e-01	-0.354	-0.506	-0.152
0.30					
NaSO4-	2.086e-03	1.387e-03	-2.681	-2.858	-0.177
20.50					
NaCO3-	1.702e-04	1.254e-04	-3.769	-3.902	-0.133
4.47					
NaHCO3	8.875e-05	1.037e-04	-4.052	-3.984	0.067
1.80					
NaOH	2.142e-16	2.501e-16	-15.669	-15.602	0.067
(0)					
O(0)	1.984e-30				
O2	9.921e-31	1.159e-30	-30.003	-29.936	0.067
31.88					
S(6)	1.100e-02				
SO4-2	4.516e-03	7.707e-04	-2.345	-3.113	-0.768
19.78					
MgSO4	3.305e-03	3.860e-03	-2.481	-2.413	0.067
6.51					
NaSO4-	2.086e-03	1.387e-03	-2.681	-2.858	-0.177
20.50					
CaSO4	1.094e-03	1.278e-03	-2.961	-2.894	0.067
8.17					
HSO4-	1.134e-09	8.355e-10	-8.945	-9.078	-0.133
42.08					
CaHSO4+	1.076e-10	7.927e-11	-9.968	-10.101	-0.133
(0)					

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

Phase	SI**	log IAP	log K(322 K,	1 atm)
Anhydrite	-0.65	-5.22	-4.56	CaSO4
Aragonite	1.27	-7.26	-8.53	CaCO3
Calcite	1.40	-7.26	-8.65	CaCO3
CO2(g)	-3.38	-5.08	-1.70	CO2
Dolomite	3.28	-14.33	-17.61	CaMg(CO3)2
Gypsum	-0.62	-5.23	-4.62	CaSO4:2H2O
H2(g)	-24.51	-27.65	-3.14	H2
H2O(g)	-0.95	-0.01	0.94	H2O
Halite	-2.54	-0.96	1.59	NaCl
O2(g)	-26.91	-29.94	-3.03	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
C	1.864e-03	1.864e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	8.180	Charge balance
	pe =	7.913	Adjusted to redox
equilibrium			
Specific Conductance ($\mu\text{S}/\text{cm}$, 49°C)	=	77930	
Density (g/cm^3)	=	1.01510	
Volume (L)	=	1.01887	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.742e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	2.400e-03	
Total CO2 (mol/kg)	=	1.864e-03	
Temperature (°C)	=	49.00	
Pressure (atm)	=	61.24	
Electrical balance (eq)	=	1.460e-02	
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23	
Iterations	=	10	
Total H	=	1.110139e+02	
Total O	=	5.555589e+01	

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	Gamma
			Molality	Activity		
OH-	1.342e-05	8.023e-06	-4.872	-5.096	-0.223	-
2.20						
H+	8.834e-09	6.605e-09	-8.054	-8.180	-0.126	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.18						
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-112.647	-112.579	0.067	
37.30						
C(4)	1.864e-03					
HCO3-	9.992e-04	6.655e-04	-3.000	-3.177	-0.176	
27.92						
MgHCO3+	1.795e-04	1.110e-04	-3.746	-3.955	-0.209	
6.45						
NaCO3-	1.705e-04	1.257e-04	-3.768	-3.901	-0.132	
4.98						

CaCO3	1.523e-04	1.778e-04	-3.817	-3.750	0.067	-
14.13						
CaHCO3+	1.242e-04	8.485e-05	-3.906	-4.071	-0.166	
10.76						
MgCO3	1.011e-04	1.180e-04	-3.995	-3.928	0.067	-
16.66						
NaHCO3	9.380e-05	1.096e-04	-4.028	-3.960	0.067	
1.80						
CO3-2	3.631e-05	7.146e-06	-4.440	-5.146	-0.706	-
1.50						
CO2	6.990e-06	8.164e-06	-5.156	-5.088	0.067	
35.54						
(CO2) 2	2.090e-12	2.441e-12	-11.680	-11.612	0.067	
71.09						
Ca	3.500e-02					
Ca+2	3.363e-02	7.932e-03	-1.473	-2.101	-0.627	-
16.02						
CaSO4	1.095e-03	1.278e-03	-2.961	-2.893	0.067	
8.31						
CaCO3	1.523e-04	1.778e-04	-3.817	-3.750	0.067	-
14.13						
CaHCO3+	1.242e-04	8.485e-05	-3.906	-4.071	-0.166	
10.76						
CaOH+	2.665e-07	1.965e-07	-6.574	-6.707	-0.132	
(0)						
CaHSO4+	1.147e-10	8.462e-11	-9.940	-10.073	-0.132	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.544e-01	-0.243	-0.450	-0.208	
19.10						
H(0)	5.935e-36					
H2	2.968e-36	3.466e-36	-35.528	-35.460	0.067	
28.56						
Mg	4.800e-02					
Mg+2	4.436e-02	1.212e-02	-1.353	-1.916	-0.563	-
20.61						
MgSO4	3.286e-03	3.838e-03	-2.483	-2.416	0.067	
6.65						
MgHCO3+	1.795e-04	1.110e-04	-3.746	-3.955	-0.209	
6.45						
MgCO3	1.011e-04	1.180e-04	-3.995	-3.928	0.067	-
16.66						
MgOH+	6.944e-05	4.833e-05	-4.158	-4.316	-0.157	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.124e-01	-0.354	-0.505	-0.151	
0.48						
NaSO4-	2.099e-03	1.398e-03	-2.678	-2.855	-0.176	
20.12						
NaCO3-	1.705e-04	1.257e-04	-3.768	-3.901	-0.132	
4.98						
NaHCO3	9.380e-05	1.096e-04	-4.028	-3.960	0.067	
1.80						
NaOH	2.138e-16	2.497e-16	-15.670	-15.603	0.067	
(0)						
O(0)	7.479e-15					

O2	3.739e-15	4.367e-15	-14.427	-14.360	0.067
31.74					
S(-2)	0.000e+00				
HS-	0.000e+00	0.000e+00	-109.486	-109.709	-0.223
22.05					
H2S	0.000e+00	0.000e+00	-111.277	-111.209	0.067
37.12					
S-2	0.000e+00	0.000e+00	-113.026	-113.765	-0.739
(0)					
S(6)	1.100e-02				
SO4-2	4.520e-03	7.756e-04	-2.345	-3.110	-0.766
19.58					
MgSO4	3.286e-03	3.838e-03	-2.483	-2.416	0.067
6.65					
NaSO4-	2.099e-03	1.398e-03	-2.678	-2.855	-0.176
20.12					
CaSO4	1.095e-03	1.278e-03	-2.961	-2.893	0.067
8.31					
HSO4-	1.134e-09	8.365e-10	-8.945	-9.078	-0.132
41.91					
CaHSO4+	1.147e-10	8.462e-11	-9.940	-10.073	-0.132
(0)					

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

Phase	SI**	log IAP	log K(322 K, 61 atm)	
Anhydrite	-0.69	-5.21	-4.52	CaSO4
Aragonite	1.23	-7.25	-8.48	CaCO3
Calcite	1.35	-7.25	-8.60	CaCO3
CH4(g)	-109.59	-112.58	-2.99	CH4
CO2(g)	-3.35	-5.09	-1.74	CO2
Dolomite	3.19	-14.31	-17.50	CaMg(CO3)2
Gypsum	-0.64	-5.23	-4.58	CaSO4:2H2O
H2(g)	-32.30	-35.46	-3.16	H2
H2O(g)	-0.93	-0.01	0.92	H2O
H2S(g)	-109.92	-117.89	-7.97	H2S
Halite	-2.55	-0.96	1.60	NaCl
O2(g)	-11.30	-14.36	-3.06	O2
Sulfur	-83.35	-79.02	4.33	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

 Reading input data for simulation 2.

 End of Run after 0.135 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=50.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=50.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 50
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
61.24

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01

Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

--

	pH	=	8.200
	pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 50°C)		=	79144
Density (g/cm^3)		=	1.01210
Volume (L)		=	1.02188
Activity of water		=	0.981
Ionic strength (mol/kgw)		=	6.741e-01
Mass of water (kg)		=	1.000e+00
Total carbon (mol/kg)		=	1.849e-03
Total CO2 (mol/kg)		=	1.849e-03
Temperature (°C)		=	50.00
Electrical balance (eq)		=	1.460e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$		=	1.23
	Iterations	=	7
	Total H	=	1.110139e+02
	Total O	=	5.555585e+01

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	1.427e-05	8.512e-06	-4.846	-5.070	-0.224	-
2.12						
H+	8.451e-09	6.310e-09	-8.073	-8.200	-0.127	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.23						
C(4)	1.849e-03					
HCO3-	9.895e-04	6.578e-04	-3.005	-3.182	-0.177	
27.88						
MgHCO3+	1.774e-04	1.094e-04	-3.751	-3.961	-0.210	
6.29						
NaCO3-	1.760e-04	1.296e-04	-3.754	-3.887	-0.133	
4.50						
CaCO3	1.533e-04	1.790e-04	-3.815	-3.747	0.067	-
14.53						
CaHCO3+	1.224e-04	8.344e-05	-3.912	-4.079	-0.166	
10.66						
MgCO3	1.005e-04	1.174e-04	-3.998	-3.930	0.067	-
17.10						
NaHCO3	8.664e-05	1.012e-04	-4.062	-3.995	0.067	
1.80						
CO3-2	3.573e-05	6.977e-06	-4.447	-5.156	-0.709	-
2.05						
CO2	6.994e-06	8.168e-06	-5.155	-5.088	0.067	
35.66						

(CO2)2	2.145e-12	2.505e-12	-11.669	-11.601	0.067	
71.32						
Ca	3.500e-02					
Ca+2	3.364e-02	7.869e-03	-1.473	-2.104	-0.631	-
16.41						
CaSO4	1.089e-03	1.272e-03	-2.963	-2.896	0.067	
8.19						
CaCO3	1.533e-04	1.790e-04	-3.815	-3.747	0.067	-
14.53						
CaHCO3+	1.224e-04	8.344e-05	-3.912	-4.079	-0.166	
10.66						
CaOH+	2.758e-07	2.031e-07	-6.559	-6.692	-0.133	
(0)						
CaHSO4+	1.092e-10	8.043e-11	-9.962	-10.095	-0.133	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.536e-01	-0.243	-0.452	-0.209	
19.10						
H(0)	3.836e-28					
H2	1.918e-28	2.240e-28	-27.717	-27.650	0.067	
28.59						
Mg	4.800e-02					
Mg+2	4.430e-02	1.201e-02	-1.354	-1.920	-0.567	-
21.09						
MgSO4	3.339e-03	3.900e-03	-2.476	-2.409	0.067	
6.53						
MgHCO3+	1.774e-04	1.094e-04	-3.751	-3.961	-0.210	
6.29						
MgCO3	1.005e-04	1.174e-04	-3.998	-3.930	0.067	-
17.10						
MgOH+	7.837e-05	5.445e-05	-4.106	-4.264	-0.158	
(0)						
Na	4.450e-01					
Na+	4.427e-01	3.117e-01	-0.354	-0.506	-0.152	
0.32						
NaSO4-	2.080e-03	1.382e-03	-2.682	-2.859	-0.177	
20.45						
NaCO3-	1.760e-04	1.296e-04	-3.754	-3.887	-0.133	
4.50						
NaHCO3	8.664e-05	1.012e-04	-4.062	-3.995	0.067	
1.80						
NaOH	2.272e-16	2.653e-16	-15.644	-15.576	0.067	
(0)						
O(0)	3.807e-30					
O2	1.903e-30	2.223e-30	-29.720	-29.653	0.067	
31.92						
S(6)	1.100e-02					
SO4-2	4.492e-03	7.645e-04	-2.348	-3.117	-0.769	
19.83						
MgSO4	3.339e-03	3.900e-03	-2.476	-2.409	0.067	
6.53						
NaSO4-	2.080e-03	1.382e-03	-2.682	-2.859	-0.177	
20.45						
CaSO4	1.089e-03	1.272e-03	-2.963	-2.896	0.067	
8.19						
HSO4-	1.155e-09	8.502e-10	-8.938	-9.070	-0.133	
42.11						

CaHSO4+ 1.092e-10 8.043e-11 -9.962 -10.095 -0.133
 (0)

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

--

Phase	SI**	log IAP	log K(323 K,	1 atm)
Anhydrite	-0.65	-5.22	-4.58	CaSO4
Aragonite	1.28	-7.26	-8.54	CaCO3
Calcite	1.40	-7.26	-8.66	CaCO3
CO2(g)	-3.38	-5.09	-1.71	CO2
Dolomite	3.29	-14.34	-17.63	CaMg(CO3)2
Gypsum	-0.62	-5.24	-4.62	CaSO4:2H2O
H2(g)	-24.51	-27.65	-3.14	H2
H2O(g)	-0.92	-0.01	0.92	H2O
Halite	-2.55	-0.96	1.59	NaCl
O2(g)	-26.62	-29.65	-3.03	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
 Using pressure 1.

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

--

Elements	Molality	Moles
C	1.849e-03	1.849e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	8.180	Charge balance
	pe =	-2.721	Adjusted to redox
equilibrium			
	Specific Conductance (µS/cm, 50°C)	=	79066
	Density (g/cm³)	=	1.01464
	Volume (L)	=	1.01933
	Activity of water	=	0.981
	Ionic strength (mol/kgw)	=	6.741e-01
	Mass of water (kg)	=	1.000e+00
	Total alkalinity (eq/kg)	=	2.400e-03
	Total CO2 (mol/kg)	=	1.849e-03

Temperature (°C) = 50.00
 Pressure (atm) = 61.24
 Electrical balance (eq) = 1.460e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
 Iterations = 15
 Total H = 1.110139e+02
 Total O = 5.555585e+01

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

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.426e-05	8.522e-06	-4.846	-5.069	-0.224	-
2.21						
H+	8.833e-09	6.601e-09	-8.054	-8.180	-0.127	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.19						
C(-4)	1.960e-28					
CH4	1.960e-28	2.289e-28	-27.708	-27.640	0.067	
37.37						
C(4)	1.849e-03					
HCO3-	9.815e-04	6.533e-04	-3.008	-3.185	-0.177	
27.94						
MgHCO3+	1.772e-04	1.095e-04	-3.751	-3.961	-0.209	
6.46						
NaCO3-	1.764e-04	1.300e-04	-3.754	-3.886	-0.132	
5.00						
CaCO3	1.552e-04	1.812e-04	-3.809	-3.742	0.067	-
14.13						
CaHCO3+	1.224e-04	8.353e-05	-3.912	-4.078	-0.166	
10.77						
MgCO3	1.014e-04	1.184e-04	-3.994	-3.927	0.067	-
16.67						
NaHCO3	9.156e-05	1.069e-04	-4.038	-3.971	0.067	
1.80						
CO3-2	3.609e-05	7.083e-06	-4.443	-5.150	-0.707	-
1.56						
CO2	6.852e-06	8.003e-06	-5.164	-5.097	0.067	
35.59						
(CO2)2	2.059e-12	2.404e-12	-11.686	-11.619	0.067	
71.19						
Ca	3.500e-02					
Ca+2	3.363e-02	7.910e-03	-1.473	-2.102	-0.629	-
16.02						
CaSO4	1.090e-03	1.273e-03	-2.963	-2.895	0.067	
8.33						
CaCO3	1.552e-04	1.812e-04	-3.809	-3.742	0.067	-
14.13						
CaHCO3+	1.224e-04	8.353e-05	-3.912	-4.078	-0.166	
10.77						
CaOH+	2.661e-07	1.961e-07	-6.575	-6.707	-0.132	
(0)						

CaHSO4+	1.164e-10	8.582e-11	-9.934	-10.066	-0.132	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.541e-01	-0.243	-0.451	-0.208	
19.10						
H(0)	1.091e-14					
H2	5.453e-15	6.369e-15	-14.263	-14.196	0.067	
28.56						
Mg	4.800e-02					
Mg+2	4.433e-02	1.208e-02	-1.353	-1.918	-0.565	-
20.64						
MgSO4	3.320e-03	3.878e-03	-2.479	-2.411	0.067	
6.67						
MgHCO3+	1.772e-04	1.095e-04	-3.751	-3.961	-0.209	
6.46						
MgCO3	1.014e-04	1.184e-04	-3.994	-3.927	0.067	-
16.67						
MgOH+	7.482e-05	5.205e-05	-4.126	-4.284	-0.158	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.122e-01	-0.354	-0.506	-0.152	
0.50						
NaSO4-	2.093e-03	1.393e-03	-2.679	-2.856	-0.177	
20.07						
NaCO3-	1.764e-04	1.300e-04	-3.754	-3.886	-0.132	
5.00						
NaHCO3	9.156e-05	1.069e-04	-4.038	-3.971	0.067	
1.80						
NaOH	2.269e-16	2.650e-16	-15.644	-15.577	0.067	
(0)						
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-56.680	-56.613	0.067	
31.79						
S(-2)	2.903e-25					
HS-	2.857e-25	1.707e-25	-24.544	-24.768	-0.224	
22.06						
H2S	4.538e-27	5.300e-27	-26.343	-26.276	0.067	
37.13						
S-2	8.756e-29	1.594e-29	-28.058	-28.797	-0.740	
(0)						
S(6)	1.100e-02					
SO4-2	4.496e-03	7.693e-04	-2.347	-3.114	-0.767	
19.63						
MgSO4	3.320e-03	3.878e-03	-2.479	-2.411	0.067	
6.67						
NaSO4-	2.093e-03	1.393e-03	-2.679	-2.856	-0.177	
20.07						
CaSO4	1.090e-03	1.273e-03	-2.963	-2.895	0.067	
8.33						
HSO4-	1.154e-09	8.508e-10	-8.938	-9.070	-0.132	
41.93						
CaHSO4+	1.164e-10	8.582e-11	-9.934	-10.066	-0.132	
(0)						

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

Phase	SI**	log IAP	log K(323 K,	61 atm)
Anhydrite	-0.68	-5.22	-4.53	CaSO4
Aragonite	1.23	-7.25	-8.48	CaCO3
Calcite	1.36	-7.25	-8.61	CaCO3
CH4(g)	-24.64	-27.64	-3.00	CH4
CO2(g)	-3.35	-5.10	-1.75	CO2
Dolomite	3.20	-14.32	-17.52	CaMg(CO3)2
Gypsum	-0.65	-5.23	-4.59	CaSO4:2H2O
H2(g)	-11.03	-14.20	-3.16	H2
H2O(g)	-0.91	-0.01	0.90	H2O
H2S(g)	-24.98	-32.95	-7.97	H2S
Halite	-2.55	-0.96	1.60	NaCl
O2(g)	-53.55	-56.61	-3.06	O2
Sulfur	-19.66	-15.36	4.31	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.073 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=55.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=55.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 55
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
61.24

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 55°C)	=	84902
Density (g/cm^3)	=	1.00970
Volume (L)	=	1.02431
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.735e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.768e-03
Total CO2 (mol/kg)	=	1.768e-03
Temperature (°C)	=	55.00
Electrical balance (eq)	=	1.460e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23
Iterations	=	8
Total H	=	1.110138e+02
Total O	=	5.555565e+01

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

--

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.917e-05	1.138e-05	-4.717	-4.944	-0.226	-
2.14						
H+	8.472e-09	6.310e-09	-8.072	-8.200	-0.128	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.28						
C(4)	1.768e-03					
HCO3-	9.003e-04	5.963e-04	-3.046	-3.224	-0.179	
27.94						
NaCO3-	2.050e-04	1.504e-04	-3.688	-3.823	-0.134	
4.60						
CaCO3	1.666e-04	1.946e-04	-3.778	-3.711	0.067	-
14.52						
MgHCO3+	1.660e-04	1.020e-04	-3.780	-3.992	-0.212	
6.33						
CaHCO3+	1.126e-04	7.653e-05	-3.948	-4.116	-0.168	
10.75						
MgCO3	1.006e-04	1.174e-04	-3.998	-3.930	0.067	-
17.10						
NaHCO3	7.639e-05	8.921e-05	-4.117	-4.050	0.067	
1.80						
CO3-2	3.418e-05	6.582e-06	-4.466	-5.182	-0.715	-
2.40						
CO2	6.347e-06	7.412e-06	-5.197	-5.130	0.067	
35.92						
(CO2)2	1.990e-12	2.324e-12	-11.701	-11.634	0.067	
71.84						
Ca	3.500e-02					
Ca+2	3.366e-02	7.756e-03	-1.473	-2.110	-0.637	-
16.42						
CaSO4	1.064e-03	1.242e-03	-2.973	-2.906	0.067	
8.29						
CaCO3	1.666e-04	1.946e-04	-3.778	-3.711	0.067	-
14.52						
CaHCO3+	1.126e-04	7.653e-05	-3.948	-4.116	-0.168	
10.75						
CaOH+	2.727e-07	2.002e-07	-6.564	-6.699	-0.134	
(0)						
CaHSO4+	1.181e-10	8.666e-11	-9.928	-10.062	-0.134	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.520e-01	-0.243	-0.453	-0.211	
19.06						
H(0)	3.680e-28					
H2	1.840e-28	2.148e-28	-27.735	-27.668	0.067	
28.58						
Mg	4.800e-02					
Mg+2	4.411e-02	1.179e-02	-1.355	-1.928	-0.573	-
21.23						

MgSO4	3.508e-03	4.096e-03	-2.455	-2.388	0.067	
6.63						
MgHCO3+	1.660e-04	1.020e-04	-3.780	-3.992	-0.212	
6.33						
MgOH+	1.127e-04	7.804e-05	-3.948	-4.108	-0.159	
(0)						
MgCO3	1.006e-04	1.174e-04	-3.998	-3.930	0.067	-
17.10						
Na	4.450e-01					
Na+	4.427e-01	3.104e-01	-0.354	-0.508	-0.154	
0.43						
NaSO4-	2.050e-03	1.358e-03	-2.688	-2.867	-0.179	
20.15						
NaCO3-	2.050e-04	1.504e-04	-3.688	-3.823	-0.134	
4.60						
NaHCO3	7.639e-05	8.921e-05	-4.117	-4.050	0.067	
1.80						
NaOH	3.026e-16	3.533e-16	-15.519	-15.452	0.067	
(0)						
O(0)	9.323e-29					
O2	4.662e-29	5.444e-29	-28.331	-28.264	0.067	
32.16						
S(6)	1.100e-02					
SO4-2	4.379e-03	7.343e-04	-2.359	-3.134	-0.775	
20.02						
MgSO4	3.508e-03	4.096e-03	-2.455	-2.388	0.067	
6.63						
NaSO4-	2.050e-03	1.358e-03	-2.688	-2.867	-0.179	
20.15						
CaSO4	1.064e-03	1.242e-03	-2.973	-2.906	0.067	
8.29						
HSO4-	1.266e-09	9.293e-10	-8.898	-9.032	-0.134	
42.23						
CaHSO4+	1.181e-10	8.666e-11	-9.928	-10.062	-0.134	
(0)						

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

Phase	SI**	log IAP	log K(328 K,	1 atm)
Anhydrite	-0.60	-5.24	-4.64	CaSO4
Aragonite	1.29	-7.29	-8.59	CaCO3
Calcite	1.42	-7.29	-8.71	CaCO3
CO2(g)	-3.38	-5.13	-1.75	CO2
Dolomite	3.32	-14.40	-17.72	CaMg(CO3)2
Gypsum	-0.63	-5.26	-4.63	CaSO4:2H2O
H2(g)	-24.53	-27.67	-3.14	H2
H2O(g)	-0.82	-0.01	0.81	H2O
Halite	-2.55	-0.96	1.59	NaCl
O2(g)	-25.22	-28.26	-3.05	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.

Using pressure 1.

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

Elements	Molality	Moles
C	1.768e-03	1.768e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

	pH =	8.182	Charge balance
	pe =	-2.495	Adjusted to redox
equilibrium			
Specific Conductance ($\mu\text{S}/\text{cm}$, 55°C)	=	84782	
Density (g/cm^3)	=	1.01224	
Volume (L)	=	1.02174	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.735e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	2.400e-03	
Total CO2 (mol/kg)	=	1.768e-03	
Temperature (°C)	=	55.00	
Pressure (atm)	=	61.24	
Electrical balance (eq)	=	1.460e-02	
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23	
Iterations	=	14	
Total H	=	1.110138e+02	
Total O	=	5.555565e+01	

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

mole V Species cm^3/mol	Molality	Activity	Log		Log	
			Molality	Activity	Gamma	
OH-	1.922e-05	1.143e-05	-4.716	-4.942	-0.226	-
2.26						
H+	8.825e-09	6.578e-09	-8.054	-8.182	-0.128	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.23						
C(-4)	6.533e-31					

CH4	6.533e-31	7.630e-31	-30.185	-30.118	0.067	
37.70						
C(4)	1.768e-03					
HCO3-	8.921e-04	5.917e-04	-3.050	-3.228	-0.178	
28.01						
NaCO3-	2.057e-04	1.511e-04	-3.687	-3.821	-0.134	
5.09						
CaCO3	1.690e-04	1.974e-04	-3.772	-3.705	0.067	-
14.13						
MgHCO3+	1.656e-04	1.019e-04	-3.781	-3.992	-0.211	
6.49						
CaHCO3+	1.125e-04	7.654e-05	-3.949	-4.116	-0.167	
10.86						
MgCO3	1.015e-04	1.186e-04	-3.993	-3.926	0.067	-
16.67						
NaHCO3	8.061e-05	9.413e-05	-4.094	-4.026	0.067	
1.80						
CO3-2	3.460e-05	6.697e-06	-4.461	-5.174	-0.713	-
1.89						
CO2	6.195e-06	7.234e-06	-5.208	-5.141	0.067	
35.85						
(CO2)2	1.895e-12	2.213e-12	-11.722	-11.655	0.067	
71.69						
Ca	3.500e-02					
Ca+2	3.365e-02	7.798e-03	-1.473	-2.108	-0.635	-
16.02						
CaSO4	1.065e-03	1.244e-03	-2.973	-2.905	0.067	
8.42						
CaCO3	1.690e-04	1.974e-04	-3.772	-3.705	0.067	-
14.13						
CaHCO3+	1.125e-04	7.654e-05	-3.949	-4.116	-0.167	
10.86						
CaOH+	2.640e-07	1.940e-07	-6.578	-6.712	-0.134	
(0)						
CaHSO4+	1.255e-10	9.217e-11	-9.902	-10.035	-0.134	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.526e-01	-0.243	-0.453	-0.210	
19.07						
H(0)	3.670e-15					
H2	1.835e-15	2.143e-15	-14.736	-14.669	0.067	
28.56						
Mg	4.800e-02					
Mg+2	4.414e-02	1.186e-02	-1.355	-1.926	-0.571	-
20.78						
MgSO4	3.488e-03	4.074e-03	-2.457	-2.390	0.067	
6.77						
MgHCO3+	1.656e-04	1.019e-04	-3.781	-3.992	-0.211	
6.49						
MgOH+	1.079e-04	7.485e-05	-3.967	-4.126	-0.159	
(0)						
MgCO3	1.015e-04	1.186e-04	-3.993	-3.926	0.067	-
16.67						
Na	4.450e-01					
Na+	4.426e-01	3.109e-01	-0.354	-0.507	-0.153	
0.61						

NaSO4-	2.065e-03	1.370e-03	-2.685	-2.863	-0.178
19.79					
NaCO3-	2.057e-04	1.511e-04	-3.687	-3.821	-0.134
5.09					
NaHCO3	8.061e-05	9.413e-05	-4.094	-4.026	0.067
1.80					
NaOH	3.031e-16	3.540e-16	-15.518	-15.451	0.067
(0)					
O(0)	0.000e+00				
O2	0.000e+00	0.000e+00	-54.380	-54.313	0.067
32.02					
S(-2)	1.012e-27				
HS-	9.968e-28	5.929e-28	-27.001	-27.227	-0.226
22.10					
H2S	1.449e-29	1.693e-29	-28.839	-28.771	0.067
37.14					
S-2	4.124e-31	7.399e-32	-30.385	-31.131	-0.746
(0)					
S(6)	1.100e-02				
SO4-2	4.381e-03	7.387e-04	-2.358	-3.132	-0.773
19.84					
MgSO4	3.488e-03	4.074e-03	-2.457	-2.390	0.067
6.77					
NaSO4-	2.065e-03	1.370e-03	-2.685	-2.863	-0.178
19.79					
CaSO4	1.065e-03	1.244e-03	-2.973	-2.905	0.067
8.42					
HSO4-	1.262e-09	9.275e-10	-8.899	-9.033	-0.134
42.05					
CaHSO4+	1.255e-10	9.217e-11	-9.902	-10.035	-0.134
(0)					

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

Phase	SI**	log IAP	log K(328 K, 61 atm)	
Anhydrite	-0.64	-5.24	-4.60	CaSO4
Aragonite	1.25	-7.28	-8.53	CaCO3
Calcite	1.37	-7.28	-8.66	CaCO3
CH4(g)	-27.10	-30.12	-3.01	CH4
CO2(g)	-3.36	-5.14	-1.78	CO2
Dolomite	3.24	-14.38	-17.62	CaMg(CO3)2
Gypsum	-0.65	-5.26	-4.60	CaSO4:2H2O
H2(g)	-11.50	-14.67	-3.17	H2
H2O(g)	-0.80	-0.01	0.79	H2O
H2S(g)	-27.45	-35.41	-7.96	H2S
Halite	-2.56	-0.96	1.60	NaCl
O2(g)	-51.23	-54.31	-3.08	O2
Sulfur	-21.61	-17.40	4.21	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.152 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=60.pqi

Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=60.pqi

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 60
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
61.24

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 60°C)	=	90709
Density (g/cm^3)	=	1.00716
Volume (L)	=	1.02689
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.729e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.679e-03
Total CO2 (mol/kg)	=	1.679e-03
Temperature (°C)	=	60.00
Electrical balance (eq)	=	1.460e-02
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.24
Iterations	=	8
Total H	=	1.110138e+02
Total O	=	5.555543e+01

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

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	2.541e-05	1.501e-05	-4.595	-4.824	-0.228	-
2.18 H+	8.493e-09	6.310e-09	-8.071	-8.200	-0.129	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.32 C(4)	1.679e-03					
HCO3-	8.099e-04	5.345e-04	-3.092	-3.272	-0.180	
27.97 NaCO3-	2.323e-04	1.699e-04	-3.634	-3.770	-0.136	
4.64 CaCO3	1.780e-04	2.078e-04	-3.750	-3.682	0.067	-
14.51 MgHCO3+	1.540e-04	9.418e-05	-3.813	-4.026	-0.214	
6.36						

CaHCO3+	1.022e-04	6.921e-05	-3.991	-4.160	-0.169	
10.82						
MgCO3	9.846e-05	1.150e-04	-4.007	-3.939	0.067	-
17.09						
NaHCO3	6.663e-05	7.779e-05	-4.176	-4.109	0.067	
1.80						
CO3-2	3.206e-05	6.084e-06	-4.494	-5.216	-0.722	-
2.84						
CO2	5.744e-06	6.707e-06	-5.241	-5.173	0.067	
36.19						
(CO2) 2	1.822e-12	2.128e-12	-11.739	-11.672	0.067	
72.38						
Ca	3.500e-02					
Ca+2	3.368e-02	7.642e-03	-1.473	-2.117	-0.644	-
16.44						
CaSO4	1.038e-03	1.212e-03	-2.984	-2.916	0.067	
8.37						
CaCO3	1.780e-04	2.078e-04	-3.750	-3.682	0.067	-
14.51						
CaHCO3+	1.022e-04	6.921e-05	-3.991	-4.160	-0.169	
10.82						
CaOH+	2.696e-07	1.972e-07	-6.569	-6.705	-0.136	
(0)						
CaHSO4+	1.280e-10	9.361e-11	-9.893	-10.029	-0.136	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.503e-01	-0.243	-0.456	-0.213	
19.00						
H(0)	3.534e-28					
H2	1.767e-28	2.063e-28	-27.753	-27.685	0.067	
28.58						
Mg	4.800e-02					
Mg+2	4.392e-02	1.157e-02	-1.357	-1.937	-0.579	-
21.38						
MgSO4	3.671e-03	4.286e-03	-2.435	-2.368	0.067	
6.72						
MgOH+	1.601e-04	1.105e-04	-3.796	-3.957	-0.161	
(0)						
MgHCO3+	1.540e-04	9.418e-05	-3.813	-4.026	-0.214	
6.36						
MgCO3	9.846e-05	1.150e-04	-4.007	-3.939	0.067	-
17.09						
Na	4.450e-01					
Na+	4.427e-01	3.090e-01	-0.354	-0.510	-0.156	
0.54						
NaSO4-	2.019e-03	1.332e-03	-2.695	-2.875	-0.180	
19.82						
NaCO3-	2.323e-04	1.699e-04	-3.634	-3.770	-0.136	
4.64						
NaHCO3	6.663e-05	7.779e-05	-4.176	-4.109	0.067	
1.80						
NaOH	3.973e-16	4.639e-16	-15.401	-15.334	0.067	
(0)						
O(0)	2.074e-27					
O2	1.037e-27	1.211e-27	-26.984	-26.917	0.067	
32.38						
S(6)	1.100e-02					

SO4-2	4.271e-03	7.054e-04	-2.369	-3.152	-0.782
20.15					
MgSO4	3.671e-03	4.286e-03	-2.435	-2.368	0.067
6.72					
NaSO4-	2.019e-03	1.332e-03	-2.695	-2.875	-0.180
19.82					
CaSO4	1.038e-03	1.212e-03	-2.984	-2.916	0.067
8.37					
HSO4-	1.393e-09	1.019e-09	-8.856	-8.992	-0.136
42.31					
CaHSO4+	1.280e-10	9.361e-11	-9.893	-10.029	-0.136
(0)					

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

--

Phase	SI**	log IAP	log K(333 K,	1 atm)
Anhydrite	-0.56	-5.27	-4.71	CaSO4
Aragonite	1.30	-7.33	-8.64	CaCO3
Calcite	1.43	-7.33	-8.76	CaCO3
CO2 (g)	-3.39	-5.17	-1.78	CO2
Dolomite	3.33	-14.49	-17.82	CaMg (CO3) 2
Gypsum	-0.63	-5.28	-4.65	CaSO4:2H2O
H2 (g)	-24.55	-27.69	-3.14	H2
H2O (g)	-0.72	-0.01	0.71	H2O
Halite	-2.56	-0.97	1.60	NaCl
O2 (g)	-23.85	-26.92	-3.06	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

--

Elements	Molality	Moles
C	1.679e-03	1.679e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

pH = 8.184 Charge balance

```

pe = 7.318 Adjusted to redox
equilibrium
Specific Conductance (µS/cm, 60°C) = 90546
Density (g/cm³) = 1.00971
Volume (L) = 1.02429
Activity of water = 0.981
Ionic strength (mol/kgw) = 6.729e-01
Mass of water (kg) = 1.000e+00
Total alkalinity (eq/kg) = 2.400e-03
Total CO2 (mol/kg) = 1.679e-03
Temperature (°C) = 60.00
Pressure (atm) = 61.24
Electrical balance (eq) = 1.460e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.24
Iterations = 10
Total H = 1.110138e+02
Total O = 5.555543e+01

```

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

mole V Species cm³/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	2.555e-05	1.513e-05	-4.593	-4.820	-0.228	-
2.34 H+	8.813e-09	6.553e-09	-8.055	-8.184	-0.129	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.28 C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-109.353	-109.286	0.067	
38.04 C(4)	1.679e-03					
HCO3-	8.015e-04	5.297e-04	-3.096	-3.276	-0.180	
28.04 NaCO3-	2.336e-04	1.711e-04	-3.632	-3.767	-0.135	
5.13 CaCO3	1.809e-04	2.112e-04	-3.743	-3.675	0.067	-
14.12 MgHCO3+	1.534e-04	9.400e-05	-3.814	-4.027	-0.213	
6.52 CaHCO3+	1.019e-04	6.913e-05	-3.992	-4.160	-0.169	
10.93 MgCO3	9.959e-05	1.163e-04	-4.002	-3.934	0.067	-
16.67 NaHCO3	7.017e-05	8.193e-05	-4.154	-4.087	0.067	
1.80 CO3-2	3.253e-05	6.206e-06	-4.488	-5.207	-0.719	-
2.32 CO2	5.578e-06	6.513e-06	-5.253	-5.186	0.067	
36.11 (CO2)2	1.719e-12	2.007e-12	-11.765	-11.697	0.067	
72.22 Ca	3.500e-02					

Ca ²⁺	3.368e-02	7.685e-03	-1.473	-2.114	-0.642	-
16.04						
CaSO ₄	1.040e-03	1.214e-03	-2.983	-2.916	0.067	
8.51						
CaCO ₃	1.809e-04	2.112e-04	-3.743	-3.675	0.067	-
14.12						
CaHCO ₃ ⁺	1.019e-04	6.913e-05	-3.992	-4.160	-0.169	
10.93						
CaOH ⁺	2.621e-07	1.919e-07	-6.582	-6.717	-0.135	
(0)						
CaHSO ₄ ⁺	1.355e-10	9.920e-11	-9.868	-10.003	-0.135	
(0)						
Cl	5.720e-01					
Cl ⁻	5.720e-01	3.509e-01	-0.243	-0.455	-0.212	
19.01						
H(0)	8.261e-35					
H ₂	4.130e-35	4.823e-35	-34.384	-34.317	0.067	
28.55						
Mg	4.800e-02					
Mg ²⁺	4.394e-02	1.164e-02	-1.357	-1.934	-0.577	-
20.93						
MgSO ₄	3.651e-03	4.263e-03	-2.438	-2.370	0.067	
6.85						
MgOH ⁺	1.540e-04	1.064e-04	-3.813	-3.973	-0.160	
(0)						
MgHCO ₃ ⁺	1.534e-04	9.400e-05	-3.814	-4.027	-0.213	
6.52						
MgCO ₃	9.959e-05	1.163e-04	-4.002	-3.934	0.067	-
16.67						
Na	4.450e-01					
Na ⁺	4.427e-01	3.095e-01	-0.354	-0.509	-0.155	
0.72						
NaSO ₄ ⁻	2.037e-03	1.346e-03	-2.691	-2.871	-0.180	
19.47						
NaCO ₃ ⁻	2.336e-04	1.711e-04	-3.632	-3.767	-0.135	
5.13						
NaHCO ₃	7.017e-05	8.193e-05	-4.154	-4.087	0.067	
1.80						
NaOH	3.996e-16	4.665e-16	-15.398	-15.331	0.067	
(0)						
O(0)	3.379e-14					
O ₂	1.690e-14	1.973e-14	-13.772	-13.705	0.067	
32.23						
S(-2)	0.000e+00					
HS ⁻	0.000e+00	0.000e+00	-106.141	-106.368	-0.228	
22.12						
H ₂ S	0.000e+00	0.000e+00	-108.012	-107.945	0.067	
37.15						
S ⁻²	0.000e+00	0.000e+00	-109.397	-110.150	-0.753	
(0)						
S(6)	1.100e-02					
SO ₄ ⁻²	4.272e-03	7.095e-04	-2.369	-3.149	-0.780	
19.99						
MgSO ₄	3.651e-03	4.263e-03	-2.438	-2.370	0.067	
6.85						
NaSO ₄ ⁻	2.037e-03	1.346e-03	-2.691	-2.871	-0.180	
19.47						

CaSO4	1.040e-03	1.214e-03	-2.983	-2.916	0.067
8.51					
HSO4-	1.384e-09	1.014e-09	-8.859	-8.994	-0.135
42.13					
CaHSO4+	1.355e-10	9.920e-11	-9.868	-10.003	-0.135
(0)					

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

Phase	SI**	log IAP	log K(333 K, 61 atm)	
Anhydrite	-0.60	-5.26	-4.66	CaSO4
Aragonite	1.27	-7.32	-8.59	CaCO3
Calcite	1.38	-7.32	-8.71	CaCO3
CH4(g)	-106.26	-109.29	-3.03	CH4
CO2(g)	-3.37	-5.19	-1.82	CO2
Dolomite	3.25	-14.46	-17.72	CaMg(CO3)2
Gypsum	-0.66	-5.28	-4.62	CaSO4:2H2O
H2(g)	-31.15	-34.32	-3.17	H2
H2O(g)	-0.70	-0.01	0.69	H2O
H2S(g)	-106.59	-114.55	-7.96	H2S
Halite	-2.57	-0.96	1.60	NaCl
O2(g)	-10.61	-13.70	-3.10	O2
Sulfur	-81.06	-76.94	4.11	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.147 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=70.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=70.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 70
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
61.24

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 70°C)	=	102419
Density (g/cm^3)	=	1.00168
Volume (L)	=	1.03249
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.717e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.470e-03

Total CO2 (mol/kg) = 1.470e-03
 Temperature (°C) = 70.00
 Electrical balance (eq) = 1.460e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.24
 Iterations = 8
 Total H = 1.110137e+02
 Total O = 5.555498e+01

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

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm ³ /mol						
OH-	4.295e-05	2.513e-05	-4.367	-4.600	-0.233	-
2.36						
H+	8.539e-09	6.310e-09	-8.069	-8.200	-0.131	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.43						
C(4)	1.470e-03					
HCO3-	6.292e-04	4.121e-04	-3.201	-3.385	-0.184	
27.95						
NaCO3-	2.743e-04	1.992e-04	-3.562	-3.701	-0.139	
4.55						
CaCO3	1.900e-04	2.218e-04	-3.721	-3.654	0.067	-
14.49						
MgHCO3+	1.281e-04	7.763e-05	-3.892	-4.110	-0.218	
6.38						
MgCO3	8.813e-05	1.029e-04	-4.055	-3.988	0.067	-
17.09						
CaHCO3+	8.071e-05	5.427e-05	-4.093	-4.265	-0.172	
10.94						
NaHCO3	4.871e-05	5.686e-05	-4.312	-4.245	0.067	
1.80						
CO3-2	2.644e-05	4.863e-06	-4.578	-5.313	-0.735	-
3.99						
CO2	4.619e-06	5.391e-06	-5.335	-5.268	0.067	
36.77						
(CO2)2	1.444e-12	1.686e-12	-11.840	-11.773	0.067	
73.54						
Ca	3.500e-02					
Ca+2	3.374e-02	7.407e-03	-1.472	-2.130	-0.659	-
16.52						
CaSO4	9.863e-04	1.151e-03	-3.006	-2.939	0.067	
8.53						
CaCO3	1.900e-04	2.218e-04	-3.721	-3.654	0.067	-
14.49						
CaHCO3+	8.071e-05	5.427e-05	-4.093	-4.265	-0.172	
10.94						
CaOH+	2.632e-07	1.912e-07	-6.580	-6.719	-0.139	
(0)						
CaHSO4+	1.516e-10	1.101e-10	-9.819	-9.958	-0.139	
(0)						
Cl	5.720e-01					

Cl-	5.720e-01	3.469e-01	-0.243	-0.460	-0.217	
18.80						
H(0)	3.272e-28					
H2	1.636e-28	1.910e-28	-27.786	-27.719	0.067	
28.58						
Mg	4.800e-02					
Mg+2	4.349e-02	1.111e-02	-1.362	-1.954	-0.593	-
21.70						
MgSO4	3.980e-03	4.646e-03	-2.400	-2.333	0.067	
6.87						
MgOH+	3.123e-04	2.141e-04	-3.505	-3.669	-0.164	
(0)						
MgHCO3+	1.281e-04	7.763e-05	-3.892	-4.110	-0.218	
6.38						
MgCO3	8.813e-05	1.029e-04	-4.055	-3.988	0.067	-
17.09						
Na	4.450e-01					
Na+	4.427e-01	3.061e-01	-0.354	-0.514	-0.160	
0.72						
NaSO4-	1.957e-03	1.281e-03	-2.708	-2.892	-0.184	
19.01						
NaCO3-	2.743e-04	1.992e-04	-3.562	-3.701	-0.139	
4.55						
NaHCO3	4.871e-05	5.686e-05	-4.312	-4.245	0.067	
1.80						
NaOH	6.590e-16	7.692e-16	-15.181	-15.114	0.067	
(0)						
O(0)	7.829e-25					
O2	3.914e-25	4.569e-25	-24.407	-24.340	0.067	
32.79						
S(6)	1.100e-02					
SO4-2	4.077e-03	6.518e-04	-2.390	-3.186	-0.796	
20.21						
MgSO4	3.980e-03	4.646e-03	-2.400	-2.333	0.067	
6.87						
NaSO4-	1.957e-03	1.281e-03	-2.708	-2.892	-0.184	
19.01						
CaSO4	9.863e-04	1.151e-03	-3.006	-2.939	0.067	
8.53						
HSO4-	1.702e-09	1.236e-09	-8.769	-8.908	-0.139	
42.41						
CaHSO4+	1.516e-10	1.101e-10	-9.819	-9.958	-0.139	
(0)						

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

Phase	SI**	log IAP	log K(343 K,	1 atm)
Anhydrite	-0.48	-5.32	-4.84	CaSO4
Aragonite	1.31	-7.44	-8.75	CaCO3
Calcite	1.42	-7.44	-8.87	CaCO3
CO2(g)	-3.42	-5.27	-1.85	CO2
Dolomite	3.29	-14.71	-18.00	CaMg(CO3)2
Gypsum	-0.64	-5.33	-4.69	CaSO4:2H2O
H2(g)	-24.58	-27.72	-3.14	H2
H2O(g)	-0.52	-0.01	0.51	H2O

Halite	-2.58	-0.97	1.60	NaCl
O2(g)	-21.25	-24.34	-3.09	O2

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
 Using pressure 1.

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

Elements	Molality	Moles
C	1.470e-03	1.470e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

	pH =	8.187	Charge balance
	pe =	-2.342	Adjusted to redox
equilibrium			
Specific Conductance ($\mu\text{S}/\text{cm}$, 70°C)	=	102163	
Density (g/cm^3)	=	1.00428	
Volume (L)	=	1.02982	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.718e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	2.400e-03	
Total CO2 (mol/kg)	=	1.470e-03	
Temperature (°C)	=	70.00	
Pressure (atm)	=	61.24	
Electrical balance (eq)	=	1.460e-02	
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.24	
Iterations	=	14	
Total H	=	1.110137e+02	
Total O	=	5.555498e+01	

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

			Log	Log	Log	
mole V	Species	Molality	Activity	Molality	Activity	Gamma
cm^3/mol						

OH-	4.356e-05	2.553e-05	-4.361	-4.593	-0.232	-
2.58						
H+	8.780e-09	6.494e-09	-8.057	-8.187	-0.131	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.38						
C(-4)	4.253e-34					
CH4	4.253e-34	4.965e-34	-33.371	-33.304	0.067	
38.72						
C(4)	1.470e-03					
HCO3-	6.202e-04	4.068e-04	-3.207	-3.391	-0.183	
28.03						
NaCO3-	2.770e-04	2.014e-04	-3.557	-3.696	-0.138	
5.04						
CaCO3	1.938e-04	2.263e-04	-3.713	-3.645	0.067	-
14.11						
MgHCO3+	1.271e-04	7.716e-05	-3.896	-4.113	-0.217	
6.54						
MgCO3	8.945e-05	1.044e-04	-4.048	-3.981	0.067	-
16.68						
CaHCO3+	8.018e-05	5.399e-05	-4.096	-4.268	-0.172	
11.05						
NaHCO3	5.104e-05	5.958e-05	-4.292	-4.225	0.067	
1.80						
CO3-2	2.696e-05	4.989e-06	-4.569	-5.302	-0.733	-
3.44						
CO2	4.429e-06	5.170e-06	-5.354	-5.287	0.067	
36.67						
(CO2) 2	1.328e-12	1.550e-12	-11.877	-11.810	0.067	
73.33						
Ca	3.500e-02					
Ca+2	3.374e-02	7.452e-03	-1.472	-2.128	-0.656	-
16.12						
CaSO4	9.878e-04	1.153e-03	-3.005	-2.938	0.067	
8.65						
CaCO3	1.938e-04	2.263e-04	-3.713	-3.645	0.067	-
14.11						
CaHCO3+	8.018e-05	5.399e-05	-4.096	-4.268	-0.172	
11.05						
CaOH+	2.582e-07	1.878e-07	-6.588	-6.726	-0.138	
(0)						
CaHSO4+	1.590e-10	1.156e-10	-9.799	-9.937	-0.138	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.475e-01	-0.243	-0.459	-0.216	
18.81						
H(0)	1.574e-15					
H2	7.869e-16	9.185e-16	-15.104	-15.037	0.067	
28.55						
Mg	4.800e-02					
Mg+2	4.352e-02	1.118e-02	-1.361	-1.952	-0.590	-
21.25						
MgSO4	3.959e-03	4.621e-03	-2.402	-2.335	0.067	
6.99						
MgOH+	3.031e-04	2.081e-04	-3.518	-3.682	-0.163	
(0)						

MgHCO3+	1.271e-04	7.716e-05	-3.896	-4.113	-0.217	
6.54						
MgCO3	8.945e-05	1.044e-04	-4.048	-3.981	0.067	-
16.68						
Na	4.450e-01					
Na+	4.427e-01	3.066e-01	-0.354	-0.513	-0.159	
0.90						
NaSO4-	1.978e-03	1.297e-03	-2.704	-2.887	-0.183	
18.70						
NaCO3-	2.770e-04	2.014e-04	-3.557	-3.696	-0.138	
5.04						
NaHCO3	5.104e-05	5.958e-05	-4.292	-4.225	0.067	
1.80						
NaOH	6.683e-16	7.801e-16	-15.175	-15.108	0.067	
(0)						
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-49.821	-49.754	0.067	
32.63						
S(-2)	8.578e-31					
HS-	8.470e-31	4.964e-31	-30.072	-30.304	-0.232	
22.07						
H2S	1.001e-32	1.168e-32	-32.000	-31.933	0.067	
37.16						
S-2	8.235e-34	1.409e-34	-33.084	-33.851	-0.767	
(0)						
S(6)	1.100e-02					
SO4-2	4.076e-03	6.555e-04	-2.390	-3.183	-0.794	
20.09						
MgSO4	3.959e-03	4.621e-03	-2.402	-2.335	0.067	
6.99						
NaSO4-	1.978e-03	1.297e-03	-2.704	-2.887	-0.183	
18.70						
CaSO4	9.878e-04	1.153e-03	-3.005	-2.938	0.067	
8.65						
HSO4-	1.679e-09	1.220e-09	-8.775	-8.913	-0.138	
42.23						
CaHSO4+	1.590e-10	1.156e-10	-9.799	-9.937	-0.138	
(0)						

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

Phase	SI**	log IAP	log K(343 K,	61 atm)
Anhydrite	-0.51	-5.31	-4.80	CaSO4
Aragonite	1.27	-7.43	-8.70	CaCO3
Calcite	1.39	-7.43	-8.82	CaCO3
CH4(g)	-30.26	-33.30	-3.04	CH4
CO2(g)	-3.41	-5.29	-1.88	CO2
Dolomite	3.21	-14.68	-17.90	CaMg(CO3)2
Gypsum	-0.67	-5.33	-4.66	CaSO4:2H2O
H2(g)	-11.87	-15.04	-3.16	H2
H2O(g)	-0.51	-0.01	0.50	H2O
H2S(g)	-30.54	-38.49	-7.95	H2S
Halite	-2.58	-0.97	1.61	NaCl
O2(g)	-46.63	-49.75	-3.12	O2
Sulfur	-24.18	-20.24	3.93	S

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.155 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=80.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=80.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 80
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg

REACTION_PRESSURE 1
61.24

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

	pH	=	8.200
	pe	=	4.000
Specific Conductance	($\mu\text{S}/\text{cm}$, 80°C)	=	114163
	Density (g/cm^3)	=	0.99572
	Volume (L)	=	1.03866
	Activity of water	=	0.981
	Ionic strength (mol/kgw)	=	6.706e-01
	Mass of water (kg)	=	1.000e+00
	Total carbon (mol/kg)	=	1.198e-03
	Total CO2 (mol/kg)	=	1.198e-03
	Temperature (°C)	=	80.00
	Electrical balance (eq)	=	1.460e-02
Percent error,	$100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.24
	Iterations	=	9
	Total H	=	1.110137e+02
	Total O	=	5.555446e+01

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

mole V Species cm^3/mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	6.927e-05	4.009e-05	-4.159	-4.397	-0.238	-
2.66 H+	8.588e-09	6.310e-09	-8.066	-8.200	-0.134	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.54 C(4)	1.198e-03					
HCO3-	4.509e-04	2.928e-04	-3.346	-3.533	-0.187	
27.82						

NaCO3-	2.831e-04	2.041e-04	-3.548	-3.690	-0.142	
4.25						
CaCO3	1.797e-04	2.097e-04	-3.745	-3.678	0.067	-
14.47						
MgHCO3+	9.900e-05	5.940e-05	-4.004	-4.226	-0.222	
6.35						
MgCO3	7.023e-05	8.196e-05	-4.153	-4.086	0.067	-
17.08						
CaHCO3+	5.928e-05	3.956e-05	-4.227	-4.403	-0.176	
11.03						
NaHCO3	3.289e-05	3.838e-05	-4.483	-4.416	0.067	
1.80						
CO3-2	1.953e-05	3.476e-06	-4.709	-5.459	-0.750	-
5.50						
CO2	3.516e-06	4.103e-06	-5.454	-5.387	0.067	
37.40						
(CO2) 2	1.001e-12	1.168e-12	-12.000	-11.933	0.067	
74.80						
Ca	3.500e-02					
Ca+2	3.383e-02	7.168e-03	-1.471	-2.145	-0.674	-
16.65						
CaSO4	9.344e-04	1.090e-03	-3.029	-2.962	0.067	
8.66						
CaCO3	1.797e-04	2.097e-04	-3.745	-3.678	0.067	-
14.47						
CaHCO3+	5.928e-05	3.956e-05	-4.227	-4.403	-0.176	
11.03						
CaOH+	2.567e-07	1.850e-07	-6.591	-6.733	-0.142	
(0)						
CaHSO4+	1.815e-10	1.308e-10	-9.741	-9.883	-0.142	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.432e-01	-0.243	-0.464	-0.222	
18.51						
H(0)	3.042e-28					
H2	1.521e-28	1.775e-28	-27.818	-27.751	0.067	
28.57						
Mg	4.800e-02					
Mg+2	4.299e-02	1.062e-02	-1.367	-1.974	-0.607	-
22.04						
MgSO4	4.259e-03	4.970e-03	-2.371	-2.304	0.067	
7.00						
MgOH+	5.832e-04	3.970e-04	-3.234	-3.401	-0.167	
(0)						
MgHCO3+	9.900e-05	5.940e-05	-4.004	-4.226	-0.222	
6.35						
MgCO3	7.023e-05	8.196e-05	-4.153	-4.086	0.067	-
17.08						
Na	4.450e-01					
Na+	4.428e-01	3.031e-01	-0.354	-0.518	-0.165	
0.88						
NaSO4-	1.896e-03	1.231e-03	-2.722	-2.910	-0.187	
18.01						
NaCO3-	2.831e-04	2.041e-04	-3.548	-3.690	-0.142	
4.25						
NaHCO3	3.289e-05	3.838e-05	-4.483	-4.416	0.067	
1.80						

NaOH	1.041e-15	1.215e-15	-14.982	-14.915	0.067
(0)					
O(0)	2.111e-22				
O2	1.056e-22	1.232e-22	-21.976	-21.909	0.067
33.17					
S(6)	1.100e-02				
MgSO4	4.259e-03	4.970e-03	-2.371	-2.304	0.067
7.00					
SO4-2	3.911e-03	6.039e-04	-2.408	-3.219	-0.811
20.04					
NaSO4-	1.896e-03	1.231e-03	-2.722	-2.910	-0.187
18.01					
CaSO4	9.344e-04	1.090e-03	-3.029	-2.962	0.067
8.66					
HSO4-	2.106e-09	1.518e-09	-8.676	-8.819	-0.142
42.42					
CaHSO4+	1.815e-10	1.308e-10	-9.741	-9.883	-0.142
(0)					

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

Phase	SI**	log IAP	log K(353 K,	1 atm)
Anhydrite	-0.39	-5.36	-4.98	CaSO4
Aragonite	1.27	-7.60	-8.88	CaCO3
Calcite	1.39	-7.60	-8.99	CaCO3
CO2(g)	-3.49	-5.39	-1.90	CO2
Dolomite	3.13	-15.04	-18.17	CaMg(CO3)2
Gypsum	-0.64	-5.38	-4.74	CaSO4:2H2O
H2(g)	-24.62	-27.75	-3.13	H2
H2O(g)	-0.34	-0.01	0.33	H2O
Halite	-2.59	-0.98	1.61	NaCl
O2(g)	-18.80	-21.91	-3.11	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
C	1.198e-03	1.198e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01

S 1.100e-02 1.100e-02

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

equilibrium
pH = 8.192 Charge balance
pe = -2.982 Adjusted to redox
Specific Conductance ($\mu\text{S}/\text{cm}$, 80°C) = 113808
Density (g/cm^3) = 0.99838
Volume (L) = 1.03590
Activity of water = 0.981
Ionic strength (mol/kgw) = 6.706e-01
Mass of water (kg) = 1.000e+00
Total alkalinity (eq/kg) = 2.400e-03
Total CO2 (mol/kg) = 1.198e-03
Temperature (°C) = 80.00
Pressure (atm) = 61.24
Electrical balance (eq) = 1.460e-02
Percent error, $100 * (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = 1.24
Iterations = 10
Total H = 1.110137e+02
Total O = 5.555446e+01

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

mole V Species cm^3/mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	7.090e-05	4.112e-05	-4.149	-4.386	-0.237	-
2.91						
H+	8.745e-09	6.431e-09	-8.058	-8.192	-0.133	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.49						
C(-4)	2.924e-30					
CH4	2.924e-30	3.412e-30	-29.534	-29.467	0.067	
39.43						
C(4)	1.198e-03					
HCO3-	4.421e-04	2.876e-04	-3.355	-3.541	-0.187	
27.92						
NaCO3-	2.870e-04	2.071e-04	-3.542	-3.684	-0.142	
4.74						
CaCO3	1.838e-04	2.145e-04	-3.736	-3.669	0.067	-
14.10						
MgHCO3+	9.768e-05	5.871e-05	-4.010	-4.231	-0.221	
6.51						
MgCO3	7.147e-05	8.340e-05	-4.146	-4.079	0.067	-
16.68						
CaHCO3+	5.857e-05	3.913e-05	-4.232	-4.407	-0.175	
11.13						
NaHCO3	3.423e-05	3.995e-05	-4.466	-4.399	0.067	
1.80						

CO3-2	2.002e-05	3.585e-06	-4.699	-5.446	-0.747	-
4.89						
CO2	3.321e-06	3.876e-06	-5.479	-5.412	0.067	
37.28						
(CO2)2	8.930e-13	1.042e-12	-12.049	-11.982	0.067	
74.56						
Ca	3.500e-02					
Ca+2	3.382e-02	7.214e-03	-1.471	-2.142	-0.671	-
16.26						
CaSO4	9.359e-04	1.092e-03	-3.029	-2.962	0.067	
8.77						
CaCO3	1.838e-04	2.145e-04	-3.736	-3.669	0.067	-
14.10						
CaHCO3+	5.857e-05	3.913e-05	-4.232	-4.407	-0.175	
11.13						
CaOH+	2.543e-07	1.835e-07	-6.595	-6.736	-0.142	
(0)						
CaHSO4+	1.885e-10	1.360e-10	-9.725	-9.866	-0.142	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.439e-01	-0.243	-0.464	-0.221	
18.53						
H(0)	2.745e-14					
H2	1.372e-14	1.601e-14	-13.863	-13.795	0.067	
28.55						
Mg	4.800e-02					
Mg+2	4.302e-02	1.069e-02	-1.366	-1.971	-0.605	-
21.59						
MgSO4	4.236e-03	4.943e-03	-2.373	-2.306	0.067	
7.12						
MgOH+	5.717e-04	3.897e-04	-3.243	-3.409	-0.166	
(0)						
MgHCO3+	9.768e-05	5.871e-05	-4.010	-4.231	-0.221	
6.51						
MgCO3	7.147e-05	8.340e-05	-4.146	-4.079	0.067	-
16.68						
Na	4.450e-01					
Na+	4.428e-01	3.036e-01	-0.354	-0.518	-0.164	
1.06						
NaSO4-	1.920e-03	1.249e-03	-2.717	-2.903	-0.187	
17.74						
NaCO3-	2.870e-04	2.071e-04	-3.542	-3.684	-0.142	
4.74						
NaHCO3	3.423e-05	3.995e-05	-4.466	-4.399	0.067	
1.80						
NaOH	1.066e-15	1.244e-15	-14.972	-14.905	0.067	
(0)						
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-49.935	-49.868	0.067	
33.00						
S(-2)	8.075e-27					
HS-	7.976e-27	4.625e-27	-26.098	-26.335	-0.237	
21.94						
H2S	8.586e-29	1.002e-28	-28.066	-27.999	0.067	
37.18						
S-2	1.323e-29	2.187e-30	-28.878	-29.660	-0.782	
(0)						

S(6)	1.100e-02					
MgSO4	4.236e-03	4.943e-03	-2.373	-2.306	0.067	
7.12						
SO4-2	3.908e-03	6.073e-04	-2.408	-3.217	-0.809	
19.97						
NaSO4-	1.920e-03	1.249e-03	-2.717	-2.903	-0.187	
17.74						
CaSO4	9.359e-04	1.092e-03	-3.029	-2.962	0.067	
8.77						
HSO4-	2.059e-09	1.486e-09	-8.686	-8.828	-0.142	
42.23						
CaHSO4+	1.885e-10	1.360e-10	-9.725	-9.866	-0.142	
(0)						

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

Phase	SI**	log IAP	log K(353 K, 61 atm)	
Anhydrite	-0.42	-5.36	-4.94	CaSO4
Aragonite	1.24	-7.59	-8.83	CaCO3
Calcite	1.35	-7.59	-8.94	CaCO3
CH4(g)	-26.42	-29.47	-3.05	CH4
CO2(g)	-3.48	-5.41	-1.93	CO2
Dolomite	3.06	-15.00	-18.07	CaMg(CO3)2
Gypsum	-0.67	-5.37	-4.71	CaSO4:2H2O
H2(g)	-10.64	-13.80	-3.15	H2
H2O(g)	-0.33	-0.01	0.32	H2O
H2S(g)	-26.58	-34.53	-7.95	H2S
Halite	-2.60	-0.98	1.61	NaCl
O2(g)	-46.73	-49.87	-3.13	O2
Sulfur	-21.34	-17.58	3.76	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

 Reading input data for simulation 2.

 End of Run after 0.428 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=80.pqi
 Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=80.pqo
 Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 90
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
61.24

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH = 8.200
pe = 4.000

Specific Conductance ($\mu\text{S}/\text{cm}$, 90°C) = 125834
 Density (g/cm^3) = 0.98930
 Volume (L) = 1.04539
 Activity of water = 0.981
 Ionic strength (mol/kgw) = $6.694\text{e-}01$
 Mass of water (kg) = $1.000\text{e+}00$
 Total carbon (mol/kg) = $8.224\text{e-}04$
 Total CO_2 (mol/kg) = $8.224\text{e-}04$
 Temperature ($^\circ\text{C}$) = 90.00
 Electrical balance (eq) = $1.460\text{e-}02$
 Percent error, $100 * (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = 1.24
 Iterations = 8
 Total H = $1.110140\text{e+}02$
 Total O = $5.555383\text{e+}01$

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

--

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm^3/mol						
OH-	$1.070\text{e-}04$	$6.123\text{e-}05$	-3.971	-4.213	-0.243	-
3.06						
H+	$8.642\text{e-}09$	$6.310\text{e-}09$	-8.063	-8.200	-0.137	
0.00						
H ₂ O	$5.551\text{e+}01$	$9.812\text{e-}01$	1.744	-0.008	0.000	
18.66						
C(4)	$8.224\text{e-}04$					
HCO ₃ -	$2.717\text{e-}04$	$1.749\text{e-}04$	-3.566	-3.757	-0.191	
27.60						
NaCO ₃ -	$2.342\text{e-}04$	$1.674\text{e-}04$	-3.630	-3.776	-0.146	
3.76						
CaCO ₃	$1.363\text{e-}04$	$1.590\text{e-}04$	-3.866	-3.799	0.067	-
14.45						
MgHCO ₃ +	$6.461\text{e-}05$	$3.835\text{e-}05$	-4.190	-4.416	-0.227	
6.29						
MgCO ₃	$4.550\text{e-}05$	$5.309\text{e-}05$	-4.342	-4.275	0.067	-
17.08						
CaHCO ₃ +	$3.731\text{e-}05$	$2.469\text{e-}05$	-4.428	-4.607	-0.179	
11.09						
NaHCO ₃	$1.869\text{e-}05$	$2.181\text{e-}05$	-4.728	-4.661	0.067	
1.80						
CO ₃ -2	$1.183\text{e-}05$	$2.031\text{e-}06$	-4.927	-5.692	-0.765	-
7.36						
CO ₂	$2.302\text{e-}06$	$2.686\text{e-}06$	-5.638	-5.571	0.067	
38.10						
(CO ₂) ₂	$5.015\text{e-}13$	$5.850\text{e-}13$	-12.300	-12.233	0.067	
76.21						
Ca	$3.500\text{e-}02$					
Ca+2	$3.394\text{e-}02$	$6.926\text{e-}03$	-1.469	-2.160	-0.690	-
16.84						
CaSO ₄	$8.846\text{e-}04$	$1.032\text{e-}03$	-3.053	-2.986	0.067	
8.76						
CaCO ₃	$1.363\text{e-}04$	$1.590\text{e-}04$	-3.866	-3.799	0.067	-
14.45						

CaHCO3+	3.731e-05	2.469e-05	-4.428	-4.607	-0.179	
11.09						
CaOH+	2.501e-07	1.788e-07	-6.602	-6.748	-0.146	
(0)						
CaHSO4+	2.198e-10	1.571e-10	-9.658	-9.804	-0.146	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.393e-01	-0.243	-0.469	-0.227	
18.12						
H(0)	2.840e-28					
H2	1.420e-28	1.657e-28	-27.848	-27.781	0.067	
28.57						
Mg	4.800e-02					
Mg+2	4.234e-02	1.009e-02	-1.373	-1.996	-0.623	-
22.42						
MgSO4	4.502e-03	5.252e-03	-2.347	-2.280	0.067	
7.11						
MgOH+	1.045e-03	7.057e-04	-2.981	-3.151	-0.170	
(0)						
MgHCO3+	6.461e-05	3.835e-05	-4.190	-4.416	-0.227	
6.29						
MgCO3	4.550e-05	5.309e-05	-4.342	-4.275	0.067	-
17.08						
Na	4.450e-01					
Na+	4.429e-01	2.999e-01	-0.354	-0.523	-0.169	
1.02						
NaSO4-	1.839e-03	1.184e-03	-2.735	-2.927	-0.191	
16.80						
NaCO3-	2.342e-04	1.674e-04	-3.630	-3.776	-0.146	
3.76						
NaHCO3	1.869e-05	2.181e-05	-4.728	-4.661	0.067	
1.80						
NaOH	1.574e-15	1.836e-15	-14.803	-14.736	0.067	
(0)						
O(0)	4.184e-20					
O2	2.092e-20	2.441e-20	-19.679	-19.612	0.067	
33.54						
S(6)	1.100e-02					
MgSO4	4.502e-03	5.252e-03	-2.347	-2.280	0.067	
7.11						
SO4-2	3.774e-03	5.615e-04	-2.423	-3.251	-0.827	
19.66						
NaSO4-	1.839e-03	1.184e-03	-2.735	-2.927	-0.191	
16.80						
CaSO4	8.846e-04	1.032e-03	-3.053	-2.986	0.067	
8.76						
HSO4-	2.639e-09	1.886e-09	-8.579	-8.724	-0.146	
42.34						
CaHSO4+	2.198e-10	1.571e-10	-9.658	-9.804	-0.146	
(0)						

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

Phase	SI**	log IAP	log K(363 K, 1 atm)	
Anhydrite	-0.29	-5.41	-5.12	CaSO4

Aragonite	1.16	-7.85	-9.02	CaCO3
Calcite	1.27	-7.85	-9.12	CaCO3
CO2(g)	-3.63	-5.57	-1.94	CO2
Dolomite	2.79	-15.54	-18.33	CaMg(CO3)2
Gypsum	-0.64	-5.43	-4.79	CaSO4:2H2O
H2(g)	-24.66	-27.78	-3.12	H2
H2O(g)	-0.17	-0.01	0.16	H2O
Halite	-2.61	-0.99	1.61	NaCl
O2(g)	-16.50	-19.61	-3.11	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

--

Elements	Molality	Moles
C	8.224e-04	8.224e-04
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	8.195	Charge balance
	pe =	-3.018	Adjusted to redox
equilibrium			
	Specific Conductance (µS/cm, 90°C)	=	125375
	Density (g/cm³)	=	0.99203
	Volume (L)	=	1.04252
	Activity of water	=	0.981
	Ionic strength (mol/kgw)	=	6.694e-01
	Mass of water (kg)	=	1.000e+00
	Total alkalinity (eq/kg)	=	2.400e-03
	Total CO2 (mol/kg)	=	8.224e-04
	Temperature (°C)	=	90.00
	Pressure (atm)	=	61.24
	Electrical balance (eq)	=	1.460e-02
Percent error, 100*(Cat- An)/(Cat+ An)		=	1.24
	Iterations	=	11
	Total H	=	1.110140e+02
	Total O	=	5.555383e+01

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

--

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	1.105e-04	6.333e-05	-3.957	-4.198	-0.242	-
3.35 H+	8.724e-09	6.377e-09	-8.059	-8.195	-0.136	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.61 C(-4)	2.775e-31					
CH4	2.775e-31	3.238e-31	-30.557	-30.490	0.067	
40.18 C(4)	8.224e-04					
HCO3-	2.649e-04	1.708e-04	-3.577	-3.767	-0.191	
27.71 NaCO3-	2.380e-04	1.703e-04	-3.623	-3.769	-0.145	
4.26 CaCO3	1.396e-04	1.628e-04	-3.855	-3.788	0.067	-
14.08 MgHCO3+	6.336e-05	3.768e-05	-4.198	-4.424	-0.226	
6.45 MgCO3	4.635e-05	5.408e-05	-4.334	-4.267	0.067	-
16.67 CaHCO3+	3.664e-05	2.429e-05	-4.436	-4.615	-0.179	
11.18 NaHCO3	1.932e-05	2.254e-05	-4.714	-4.647	0.067	
1.80 CO3-2	1.217e-05	2.104e-06	-4.915	-5.677	-0.762	-
6.69 CO2	2.144e-06	2.501e-06	-5.669	-5.602	0.067	
37.96 (CO2)2	4.348e-13	5.072e-13	-12.362	-12.295	0.067	
75.92 Ca	3.500e-02					
Ca+2	3.394e-02	6.974e-03	-1.469	-2.157	-0.687	-
16.44 CaSO4	8.859e-04	1.034e-03	-3.053	-2.986	0.067	
8.88 CaCO3	1.396e-04	1.628e-04	-3.855	-3.788	0.067	-
14.08 CaHCO3+	3.664e-05	2.429e-05	-4.436	-4.615	-0.179	
11.18 CaOH+	2.499e-07	1.789e-07	-6.602	-6.747	-0.145	
(0) CaHSO4+	2.262e-10	1.619e-10	-9.646	-9.791	-0.145	
(0) Cl	5.720e-01					
Cl-	5.720e-01	3.400e-01	-0.243	-0.468	-0.226	
18.15 H(0)	2.974e-14					
H2	1.487e-14	1.735e-14	-13.828	-13.761	0.067	
28.54						

Mg	4.800e-02						
Mg+2	4.238e-02	1.017e-02	-1.373	-1.993	-0.620	-	
21.96							
MgSO4	4.476e-03	5.222e-03	-2.349	-2.282	0.067		
7.22							
MgOH+	1.033e-03	6.987e-04	-2.986	-3.156	-0.170		
(0)							
MgHCO3+	6.336e-05	3.768e-05	-4.198	-4.424	-0.226		
6.45							
MgCO3	4.635e-05	5.408e-05	-4.334	-4.267	0.067	-	
16.67							
Na	4.450e-01						
Na+	4.429e-01	3.005e-01	-0.354	-0.522	-0.168		
1.19							
NaSO4-	1.867e-03	1.204e-03	-2.729	-2.919	-0.191		
16.57							
NaCO3-	2.380e-04	1.703e-04	-3.623	-3.769	-0.145		
4.26							
NaHCO3	1.932e-05	2.254e-05	-4.714	-4.647	0.067		
1.80							
NaOH	1.624e-15	1.895e-15	-14.789	-14.722	0.067		
(0)							
O(0)	0.000e+00						
O2	0.000e+00	0.000e+00	-47.766	-47.699	0.067		
33.35							
S(-2)	1.288e-27						
HS-	1.272e-27	7.290e-28	-26.896	-27.137	-0.242		
21.72							
H2S	1.291e-29	1.506e-29	-28.889	-28.822	0.067		
37.19							
S-2	3.502e-30	5.580e-31	-29.456	-30.253	-0.798		
(0)							
S(6)	1.100e-02						
MgSO4	4.476e-03	5.222e-03	-2.349	-2.282	0.067		
7.22							
SO4-2	3.771e-03	5.650e-04	-2.424	-3.248	-0.824		
19.64							
NaSO4-	1.867e-03	1.204e-03	-2.729	-2.919	-0.191		
16.57							
CaSO4	8.859e-04	1.034e-03	-3.053	-2.986	0.067		
8.88							
HSO4-	2.561e-09	1.833e-09	-8.592	-8.737	-0.145		
42.16							
CaHSO4+	2.262e-10	1.619e-10	-9.646	-9.791	-0.145		
(0)							

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

Phase	SI**	log IAP	log K(363 K, 61 atm)	
Anhydrite	-0.32	-5.40	-5.08	CaSO4
Aragonite	1.13	-7.83	-8.97	CaCO3
Calcite	1.24	-7.83	-9.07	CaCO3
CH4 (g)	-27.44	-30.49	-3.05	CH4
CO2 (g)	-3.63	-5.60	-1.98	CO2
Dolomite	2.72	-15.50	-18.23	CaMg (CO3) 2

Gypsum	-0.66	-5.42	-4.76	CaSO4:2H2O
H2 (g)	-10.62	-13.76	-3.14	H2
H2O (g)	-0.16	-0.01	0.15	H2O
H2S (g)	-27.38	-35.33	-7.95	H2S
Halite	-2.61	-0.99	1.62	NaCl
O2 (g)	-44.56	-47.70	-3.14	O2
Sulfur	-22.07	-18.47	3.60	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.417 Seconds.

Input file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=100.pqi
Output file: C:\Users\CUPGZ\Desktop\Thesis Writing\3) Discussion\1) Phreeqc modeling\P = 61.24 atm, T variable\T=100.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 100
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1

```

Ca      35
Mg      48
Na     445
S(6)   11
Alkalinity 2.4 as HCO3-
Cl     572
water  1 # kg
REACTION PRESSURE 1
61.24

```

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

```

pH = 8.200
pe = 4.000
Specific Conductance (µS/cm, 100°C) = 137325
Density (g/cm³) = 0.98245
Volume (L) = 1.05266
Activity of water = 0.981
Ionic strength (mol/kgw) = 6.680e-01
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 2.839e-04
Total CO2 (mol/kg) = 2.839e-04
Temperature (°C) = 100.00
Electrical balance (eq) = 1.460e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.24
Iterations = 8
Total H = 1.110145e+02
Total O = 5.555302e+01

```

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

mole V Species cm ³ /mol	Molality	Activity	Log	Log	Log	-
			Molality	Activity	Gamma	
OH- 3.59	1.590e-04	8.984e-05	-3.799	-4.047	-0.248	-

H+	8.698e-09	6.310e-09	-8.061	-8.200	-0.139	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.80						
C(4)	2.839e-04					
NaCO3-	9.379e-05	6.646e-05	-4.028	-4.177	-0.150	
3.04						
HCO3-	8.284e-05	5.283e-05	-4.082	-4.277	-0.195	
27.27						
CaCO3	4.958e-05	5.783e-05	-4.305	-4.238	0.067	-
14.43						
MgHCO3+	2.135e-05	1.253e-05	-4.671	-4.902	-0.231	
6.19						
MgCO3	1.443e-05	1.683e-05	-4.841	-4.774	0.067	-
17.07						
CaHCO3+	1.222e-05	8.013e-06	-4.913	-5.096	-0.183	
11.12						
NaHCO3	5.383e-06	6.278e-06	-5.269	-5.202	0.067	
1.80						
CO3-2	3.541e-06	5.857e-07	-5.451	-6.232	-0.781	-
9.60						
CO2	7.779e-07	9.073e-07	-6.109	-6.042	0.067	
38.89						
(CO2)2	6.551e-14	7.640e-14	-13.184	-13.117	0.067	
77.78						
Ca	3.500e-02					
Ca+2	3.410e-02	6.684e-03	-1.467	-2.175	-0.708	-
17.07						
CaSO4	8.387e-04	9.782e-04	-3.076	-3.010	0.067	
8.86						
CaCO3	4.958e-05	5.783e-05	-4.305	-4.238	0.067	-
14.43						
CaHCO3+	1.222e-05	8.013e-06	-4.913	-5.096	-0.183	
11.12						
CaOH+	2.435e-07	1.725e-07	-6.614	-6.763	-0.150	
(0)						
CaHSO4+	2.692e-10	1.908e-10	-9.570	-9.719	-0.150	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.353e-01	-0.243	-0.475	-0.232	
17.63						
H(0)	2.661e-28					
H2	1.331e-28	1.552e-28	-27.876	-27.809	0.067	
28.57						
Mg	4.800e-02					
Mg+2	4.147e-02	9.516e-03	-1.382	-2.022	-0.639	-
22.83						
MgSO4	4.701e-03	5.482e-03	-2.328	-2.261	0.067	
7.20						
MgOH+	1.796e-03	1.203e-03	-2.746	-2.920	-0.174	
(0)						
MgHCO3+	2.135e-05	1.253e-05	-4.671	-4.902	-0.231	
6.19						
MgCO3	1.443e-05	1.683e-05	-4.841	-4.774	0.067	-
17.07						
Na	4.450e-01					

Na+	4.431e-01	2.966e-01	-0.353	-0.528	-0.174
1.15					
NaSO4-	1.790e-03	1.141e-03	-2.747	-2.943	-0.195
15.36					
NaCO3-	9.379e-05	6.646e-05	-4.028	-4.177	-0.150
3.04					
NaHCO3	5.383e-06	6.278e-06	-5.269	-5.202	0.067
1.80					
NaOH	2.285e-15	2.665e-15	-14.641	-14.574	0.067
(0)					
O(0)	6.245e-18				
O2	3.122e-18	3.642e-18	-17.506	-17.439	0.067
33.90					
S(6)	1.100e-02				
MgSO4	4.701e-03	5.482e-03	-2.328	-2.261	0.067
7.20					
SO4-2	3.671e-03	5.250e-04	-2.435	-3.280	-0.845
19.08					
NaSO4-	1.790e-03	1.141e-03	-2.747	-2.943	-0.195
15.36					
CaSO4	8.387e-04	9.782e-04	-3.076	-3.010	0.067
8.86					
HSO4-	3.350e-09	2.374e-09	-8.475	-8.625	-0.150
42.18					
CaHSO4+	2.692e-10	1.908e-10	-9.570	-9.719	-0.150
(0)					

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

Phase	SI**	log IAP	log K(373 K,	1 atm)
Anhydrite	-0.19	-5.45	-5.26	CaSO4
Aragonite	0.76	-8.41	-9.17	CaCO3
Calcite	0.86	-8.41	-9.27	CaCO3
CO2(g)	-4.06	-6.04	-1.98	CO2
Dolomite	1.82	-16.66	-18.48	CaMg(CO3)2
Gypsum	-0.62	-5.47	-4.85	CaSO4:2H2O
H2(g)	-24.71	-27.81	-3.10	H2
H2O(g)	-0.01	-0.01	0.00	H2O
Halite	-2.62	-1.00	1.62	NaCl
O2(g)	-14.32	-17.44	-3.11	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
C	2.839e-04	2.839e-04
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	8.198	Charge balance
	pe =	-2.927	Adjusted to redox
equilibrium			
Specific Conductance ($\mu\text{S}/\text{cm}$, 100°C)	=	136758	
Density (g/cm^3)	=	0.98525	
Volume (L)	=	1.04967	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.681e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	2.400e-03	
Total CO2 (mol/kg)	=	2.839e-04	
Temperature (°C)	=	100.00	
Pressure (atm)	=	61.24	
Electrical balance (eq)	=	1.460e-02	
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.24	
Iterations	=	12	
Total H	=	1.110145e+02	
Total O	=	5.555302e+01	

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	1.651e-04	9.350e-05	-3.782	-4.029	-0.247	-
3.88						
H+	8.727e-09	6.338e-09	-8.059	-8.198	-0.139	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.74						
C(-4)	1.462e-33					
CH4	1.462e-33	1.705e-33	-32.835	-32.768	0.067	
40.99						
C(4)	2.839e-04					
NaCO3-	9.542e-05	6.771e-05	-4.020	-4.169	-0.149	
3.57						
HCO3-	8.039e-05	5.136e-05	-4.095	-4.289	-0.195	
27.41						
CaCO3	5.076e-05	5.920e-05	-4.294	-4.228	0.067	-
14.07						

MgHCO3+	2.082e-05	1.225e-05	-4.681	-4.912	-0.231	
6.35						
MgCO3	1.469e-05	1.713e-05	-4.833	-4.766	0.067	-
16.67						
CaHCO3+	1.193e-05	7.840e-06	-4.923	-5.106	-0.182	
11.21						
NaHCO3	5.529e-06	6.448e-06	-5.257	-5.191	0.067	
1.80						
CO3-2	3.654e-06	6.087e-07	-5.437	-6.216	-0.778	-
8.85						
CO2	7.161e-07	8.351e-07	-6.145	-6.078	0.067	
38.72						
(CO2) 2	5.550e-14	6.473e-14	-13.256	-13.189	0.067	
77.43						
Ca	3.500e-02					
Ca+2	3.410e-02	6.735e-03	-1.467	-2.172	-0.704	-
16.66						
CaSO4	8.398e-04	9.795e-04	-3.076	-3.009	0.067	
8.96						
CaCO3	5.076e-05	5.920e-05	-4.294	-4.228	0.067	-
14.07						
CaHCO3+	1.193e-05	7.840e-06	-4.923	-5.106	-0.182	
11.21						
CaOH+	2.448e-07	1.737e-07	-6.611	-6.760	-0.149	
(0)						
CaHSO4+	2.752e-10	1.953e-10	-9.560	-9.709	-0.149	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.360e-01	-0.243	-0.474	-0.231	
17.68						
H(0)	1.813e-14					
H2	9.065e-15	1.057e-14	-14.043	-13.976	0.067	
28.54						
Mg	4.800e-02					
Mg+2	4.151e-02	9.593e-03	-1.382	-2.018	-0.636	-
22.36						
MgSO4	4.672e-03	5.449e-03	-2.331	-2.264	0.067	
7.31						
MgOH+	1.787e-03	1.199e-03	-2.748	-2.921	-0.173	
(0)						
MgHCO3+	2.082e-05	1.225e-05	-4.681	-4.912	-0.231	
6.35						
MgCO3	1.469e-05	1.713e-05	-4.833	-4.766	0.067	-
16.67						
Na	4.450e-01					
Na+	4.431e-01	2.973e-01	-0.354	-0.527	-0.173	
1.32						
NaSO4-	1.821e-03	1.163e-03	-2.740	-2.934	-0.195	
15.19						
NaCO3-	9.542e-05	6.771e-05	-4.020	-4.169	-0.149	
3.57						
NaHCO3	5.529e-06	6.448e-06	-5.257	-5.191	0.067	
1.80						
NaOH	2.371e-15	2.765e-15	-14.625	-14.558	0.067	
(0)						
O(0)	0.000e+00					

O2	0.000e+00	0.000e+00	-45.218	-45.151	0.067
33.70					
S(-2)	2.321e-29				
HS-	2.289e-29	1.296e-29	-28.640	-28.887	-0.247
21.42					
H2S	2.265e-31	2.642e-31	-30.645	-30.578	0.067
37.20					
S-2	1.019e-31	1.562e-32	-30.992	-31.806	-0.815
(0)					
S(6)	1.100e-02				
MgSO4	4.672e-03	5.449e-03	-2.331	-2.264	0.067
7.31					
SO4-2	3.668e-03	5.285e-04	-2.436	-3.277	-0.841
19.11					
NaSO4-	1.821e-03	1.163e-03	-2.740	-2.934	-0.195
15.19					
CaSO4	8.398e-04	9.795e-04	-3.076	-3.009	0.067
8.96					
HSO4-	3.234e-09	2.295e-09	-8.490	-8.639	-0.149
42.02					
CaHSO4+	2.752e-10	1.953e-10	-9.560	-9.709	-0.149
(0)					

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

Phase	SI**	log IAP	log K(373 K, 61 atm)	
Anhydrite	-0.22	-5.45	-5.22	CaSO4
Aragonite	0.73	-8.39	-9.12	CaCO3
Calcite	0.83	-8.39	-9.21	CaCO3
CH4(g)	-29.73	-32.77	-3.04	CH4
CO2(g)	-4.07	-6.08	-2.01	CO2
Dolomite	1.76	-16.62	-18.38	CaMg(CO3)2
Gypsum	-0.64	-5.47	-4.82	CaSO4:2H2O
H2(g)	-10.85	-13.98	-3.13	H2
H2O(g)	0.00	-0.01	-0.01	H2O
H2S(g)	-29.12	-37.09	-7.96	H2S
Halite	-2.63	-1.00	1.63	NaCl
O2(g)	-42.01	-45.15	-3.14	O2
Sulfur	-23.49	-20.04	3.45	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.747 Seconds.

Input file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\P&T pairs\T=40, 7 atm.pqi

Output file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\P&T pairs\T=40, 7 atm.pqi

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
7

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01

Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

--

	pH	=	8.200
	pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)		=	67832
Density (g/cm^3)		=	1.01647
Volume (L)		=	1.01750
Activity of water		=	0.981
Ionic strength (mol/kgw)		=	6.753e-01
Mass of water (kg)		=	1.000e+00
Total carbon (mol/kg)		=	1.989e-03
Total CO2 (mol/kg)		=	1.989e-03
Temperature (°C)		=	40.00
Electrical balance (eq)		=	1.460e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$		=	1.23
	Iterations	=	7
	Total H	=	1.110141e+02
	Total O	=	5.555622e+01

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	7.568e-06	4.553e-06	-5.121	-5.342	-0.221	-
2.19						
H+	8.413e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(4)	1.989e-03					
HCO3-	1.160e-03	7.764e-04	-2.935	-3.110	-0.174	
27.66						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
CO3-2	3.684e-05	7.386e-06	-4.434	-5.132	-0.698	-
1.66						
CO2	8.476e-06	9.902e-06	-5.072	-5.004	0.068	
35.16						

(CO2)2	2.427e-12	2.835e-12	-11.615	-11.547	0.068	
70.32						
Ca	3.500e-02					
Ca+2	3.360e-02	8.086e-03	-1.474	-2.092	-0.619	-
16.46						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
CaOH+	2.817e-07	2.087e-07	-6.550	-6.681	-0.130	
(0)						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	4.185e-28					
H2	2.093e-28	2.445e-28	-27.679	-27.612	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.244e-02	-1.350	-1.905	-0.555	-
20.81						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
MgOH+	3.650e-05	2.551e-05	-4.438	-4.593	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.142e-01	-0.354	-0.503	-0.149	
0.05						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
NaOH	1.225e-16	1.431e-16	-15.912	-15.844	0.068	
(0)						
O(0)	4.672e-33					
O2	2.336e-33	2.729e-33	-32.632	-32.564	0.068	
31.40						
S(6)	1.100e-02					
SO4-2	4.738e-03	8.290e-04	-2.324	-3.081	-0.757	
19.21						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
HSO4-	9.700e-10	7.187e-10	-9.013	-9.143	-0.130	
41.78						

CaHSO4+ 9.430e-11 6.987e-11 -10.025 -10.156 -0.130
 (0)

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

--

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.72	-5.17	-4.45	CaSO4
Aragonite	1.22	-7.22	-8.45	CaCO3
Calcite	1.36	-7.22	-8.58	CaCO3
CO2(g)	-3.38	-5.00	-1.63	CO2
Dolomite	3.16	-14.26	-17.42	CaMg(CO3)2
Gypsum	-0.59	-5.19	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-29.58	-32.56	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
 Using pressure 1.

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

--

Elements	Molality	Moles
C	1.989e-03	1.989e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	8.198	Charge balance
	pe =	8.786	Adjusted to redox
equilibrium			
Specific Conductance (µS/cm, 40°C)	=	67832	
Density (g/cm³)	=	1.01673	
Volume (L)	=	1.01724	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.753e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	2.400e-03	
Total CO2 (mol/kg)	=	1.989e-03	

Temperature (°C) = 40.00
 Pressure (atm) = 7.00
 Electrical balance (eq) = 1.460e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
 Iterations = 9
 Total H = 1.110141e+02
 Total O = 5.555622e+01

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

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm ³ /mol						
OH-	7.565e-06	4.552e-06	-5.121	-5.342	-0.221	-
2.19						
H+	8.454e-09	6.342e-09	-8.073	-8.198	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.15						
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-118.523	-118.456	0.068	
36.63						
C(4)	1.989e-03					
HCO3-	1.160e-03	7.760e-04	-2.936	-3.110	-0.174	
27.66						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.18						
CaHCO3+	1.381e-04	9.476e-05	-3.860	-4.023	-0.164	
10.45						
CaCO3	1.241e-04	1.450e-04	-3.906	-3.839	0.068	-
14.52						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.051	-0.130	
4.16						
NaHCO3	1.089e-04	1.273e-04	-3.963	-3.895	0.068	
1.80						
MgCO3	9.456e-05	1.105e-04	-4.024	-3.957	0.068	-
17.05						
CO3-2	3.686e-05	7.395e-06	-4.433	-5.131	-0.698	-
1.61						
CO2	8.464e-06	9.887e-06	-5.072	-5.005	0.068	
35.15						
(CO2)2	2.420e-12	2.827e-12	-11.616	-11.549	0.068	
70.31						
Ca	3.500e-02					
Ca+2	3.360e-02	8.090e-03	-1.474	-2.092	-0.618	-
16.42						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.98						
CaHCO3+	1.381e-04	9.476e-05	-3.860	-4.023	-0.164	
10.45						
CaCO3	1.241e-04	1.450e-04	-3.906	-3.839	0.068	-
14.52						
CaOH+	2.805e-07	2.078e-07	-6.552	-6.682	-0.130	
(0)						

CaHSO4+	9.495e-11	7.035e-11	-10.023	-10.153	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	1.124e-37					
H2	5.620e-38	6.565e-38	-37.250	-37.183	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.245e-02	-1.350	-1.905	-0.555	-
20.76						
MgSO4	2.988e-03	3.491e-03	-2.525	-2.457	0.068	
6.32						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.18						
MgCO3	9.456e-05	1.105e-04	-4.024	-3.957	0.068	-
17.05						
MgOH+	3.631e-05	2.538e-05	-4.440	-4.595	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.143e-01	-0.354	-0.503	-0.149	
0.07						
NaSO4-	2.137e-03	1.430e-03	-2.670	-2.845	-0.174	
20.86						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.051	-0.130	
4.16						
NaHCO3	1.089e-04	1.273e-04	-3.963	-3.895	0.068	
1.80						
NaOH	1.224e-16	1.430e-16	-15.912	-15.845	0.068	
(0)						
O(0)	6.401e-14					
O2	3.200e-14	3.739e-14	-13.495	-13.427	0.068	
31.39						
S(-2)	0.000e+00					
HS-	0.000e+00	0.000e+00	-115.367	-115.588	-0.221	
21.90						
H2S	0.000e+00	0.000e+00	-117.082	-117.014	0.068	
37.20						
S-2	0.000e+00	0.000e+00	-119.151	-119.881	-0.730	
(0)						
S(6)	1.100e-02					
SO4-2	4.739e-03	8.296e-04	-2.324	-3.081	-0.757	
19.18						
MgSO4	2.988e-03	3.491e-03	-2.525	-2.457	0.068	
6.32						
NaSO4-	2.137e-03	1.430e-03	-2.670	-2.845	-0.174	
20.86						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.98						
HSO4-	9.704e-10	7.191e-10	-9.013	-9.143	-0.130	
41.76						
CaHSO4+	9.495e-11	7.035e-11	-10.023	-10.153	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	7 atm)	
Anhydrite	-0.73	-5.17	-4.45		CaSO4
Aragonite	1.22	-7.22	-8.44		CaCO3
Calcite	1.35	-7.22	-8.57		CaCO3
CH4(g)	-115.54	-118.46	-2.92		CH4
CO2(g)	-3.38	-5.00	-1.63		CO2
Dolomite	3.15	-14.26	-17.41		CaMg(CO3)2
Gypsum	-0.60	-5.19	-4.59		CaSO4:2H2O
H2(g)	-34.05	-37.18	-3.13		H2
H2O(g)	-1.14	-0.01	1.14		H2O
H2S(g)	-115.82	-123.79	-7.96		H2S
Halite	-2.53	-0.95	1.58		NaCl
O2(g)	-10.44	-13.43	-2.99		O2
Sulfur	-87.59	-83.05	4.54		S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.152 Seconds.

Input file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\P&T
pairs\T=41, 11 atm.pqi
Output file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\P&T
pairs\T=41, 11 atm.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 41
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
11

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 41°C)	=	68949
Density (g/cm^3)	=	1.01606
Volume (L)	=	1.01791
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.752e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.976e-03
Total CO2 (mol/kg)	=	1.976e-03
Temperature (°C)	=	41.00
Electrical balance (eq)	=	1.460e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23
Iterations	=	7
Total H	=	1.110141e+02
Total O	=	5.555618e+01

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

--

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	8.086e-06	4.861e-06	-5.092	-5.313	-0.221	-
2.18						
H+	8.416e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(4)	1.976e-03					
HCO3-	1.144e-03	7.649e-04	-2.942	-3.116	-0.175	
27.69						
MgHCO3+	1.965e-04	1.221e-04	-3.707	-3.913	-0.207	
6.18						
CaHCO3+	1.368e-04	9.383e-05	-3.864	-4.028	-0.164	
10.46						
CaCO3	1.269e-04	1.483e-04	-3.896	-3.829	0.068	-
14.56						
NaCO3-	1.252e-04	9.269e-05	-3.902	-4.033	-0.130	
4.16						
NaHCO3	1.061e-04	1.239e-04	-3.974	-3.907	0.068	
1.80						
MgCO3	9.545e-05	1.115e-04	-4.020	-3.953	0.068	-
17.10						
CO3-2	3.685e-05	7.370e-06	-4.434	-5.133	-0.699	-
1.68						
CO2	8.313e-06	9.712e-06	-5.080	-5.013	0.068	
35.21						
(CO2)2	2.400e-12	2.803e-12	-11.620	-11.552	0.068	
70.42						
Ca	3.500e-02					
Ca+2	3.360e-02	8.065e-03	-1.474	-2.093	-0.620	-
16.45						
CaSO4	1.131e-03	1.322e-03	-2.946	-2.879	0.068	
7.99						
CaHCO3+	1.368e-04	9.383e-05	-3.864	-4.028	-0.164	
10.46						
CaCO3	1.269e-04	1.483e-04	-3.896	-3.829	0.068	-
14.56						
CaOH+	2.811e-07	2.081e-07	-6.551	-6.682	-0.130	
(0)						
CaHSO4+	9.565e-11	7.082e-11	-10.019	-10.150	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.563e-01	-0.243	-0.448	-0.206	
19.09						
H(0)	4.148e-28					
H2	2.074e-28	2.423e-28	-27.683	-27.616	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.464e-02	1.240e-02	-1.350	-1.907	-0.556	-
20.84						

MgSO4	3.025e-03	3.534e-03	-2.519	-2.452	0.068	
6.33						
MgHCO3+	1.965e-04	1.221e-04	-3.707	-3.913	-0.207	
6.18						
MgCO3	9.545e-05	1.115e-04	-4.020	-3.953	0.068	-
17.10						
MgOH+	3.950e-05	2.759e-05	-4.403	-4.559	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.140e-01	-0.354	-0.503	-0.149	
0.08						
NaSO4-	2.131e-03	1.425e-03	-2.671	-2.846	-0.175	
20.86						
NaCO3-	1.252e-04	9.269e-05	-3.902	-4.033	-0.130	
4.16						
NaHCO3	1.061e-04	1.239e-04	-3.974	-3.907	0.068	
1.80						
NaOH	1.307e-16	1.526e-16	-15.884	-15.816	0.068	
(0)						
O(0)	9.310e-33					
O2	4.655e-33	5.438e-33	-32.332	-32.265	0.068	
31.46						
S(6)	1.100e-02					
SO4-2	4.713e-03	8.223e-04	-2.327	-3.085	-0.758	
19.29						
MgSO4	3.025e-03	3.534e-03	-2.519	-2.452	0.068	
6.33						
NaSO4-	2.131e-03	1.425e-03	-2.671	-2.846	-0.175	
20.86						
CaSO4	1.131e-03	1.322e-03	-2.946	-2.879	0.068	
7.99						
HSO4-	9.865e-10	7.304e-10	-9.006	-9.136	-0.130	
41.82						
CaHSO4+	9.565e-11	7.082e-11	-10.019	-10.150	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(314 K,	1 atm)
Anhydrite	-0.71	-5.18	-4.46	CaSO4
Aragonite	1.23	-7.23	-8.45	CaCO3
Calcite	1.36	-7.23	-8.59	CaCO3
CO2(g)	-3.38	-5.01	-1.63	CO2
Dolomite	3.18	-14.27	-17.44	CaMg(CO3)2
Gypsum	-0.60	-5.19	-4.60	CaSO4:2H2O
H2(g)	-24.49	-27.62	-3.13	H2
H2O(g)	-1.12	-0.01	1.12	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-29.27	-32.26	-2.99	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
C	1.976e-03	1.976e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

	pH =	8.196	Charge balance
	pe =	-2.411	Adjusted to redox
equilibrium			
Specific Conductance ($\mu\text{S}/\text{cm}$, 41°C)	=	68948	
Density (g/cm^3)	=	1.01648	
Volume (L)	=	1.01748	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.752e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	2.400e-03	
Total CO2 (mol/kg)	=	1.976e-03	
Temperature (°C)	=	41.00	
Pressure (atm)	=	11.00	
Electrical balance (eq)	=	1.460e-02	
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23	
Iterations	=	14	
Total H	=	1.110141e+02	
Total O	=	5.555618e+01	

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

mole V Species cm^3/mol	Molality	Activity	Log		Log	Gamma
			Molality	Activity		
OH-	8.080e-06	4.859e-06	-5.093	-5.313	-0.221	-
2.18						
H+	8.485e-09	6.362e-09	-8.071	-8.196	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(-4)	8.400e-30					

CH4	8.400e-30	9.813e-30	-29.076	-29.008	0.068	
36.70						
C(4)	1.976e-03					
HCO3-	1.143e-03	7.642e-04	-2.942	-3.117	-0.175	
27.69						
MgHCO3+	1.965e-04	1.222e-04	-3.707	-3.913	-0.207	
6.21						
CaHCO3+	1.369e-04	9.385e-05	-3.864	-4.028	-0.164	
10.48						
CaCO3	1.271e-04	1.485e-04	-3.896	-3.828	0.068	-
14.49						
NaCO3-	1.252e-04	9.270e-05	-3.903	-4.033	-0.130	
4.25						
NaHCO3	1.071e-04	1.251e-04	-3.970	-3.903	0.068	
1.80						
MgCO3	9.553e-05	1.116e-04	-4.020	-3.952	0.068	-
17.02						
CO3-2	3.690e-05	7.386e-06	-4.433	-5.132	-0.699	-
1.60						
CO2	8.292e-06	9.687e-06	-5.081	-5.014	0.068	
35.20						
(CO2)2	2.387e-12	2.789e-12	-11.622	-11.555	0.068	
70.40						
Ca	3.500e-02					
Ca+2	3.360e-02	8.072e-03	-1.474	-2.093	-0.619	-
16.38						
CaSO4	1.131e-03	1.322e-03	-2.946	-2.879	0.068	
8.01						
CaHCO3+	1.369e-04	9.385e-05	-3.864	-4.028	-0.164	
10.48						
CaCO3	1.271e-04	1.485e-04	-3.896	-3.828	0.068	-
14.49						
CaOH+	2.791e-07	2.067e-07	-6.554	-6.685	-0.130	
(0)						
CaHSO4+	9.673e-11	7.164e-11	-10.014	-10.145	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.564e-01	-0.243	-0.448	-0.205	
19.09						
H(0)	2.765e-15					
H2	1.383e-15	1.615e-15	-14.859	-14.792	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.465e-02	1.241e-02	-1.350	-1.906	-0.556	-
20.76						
MgSO4	3.022e-03	3.531e-03	-2.520	-2.452	0.068	
6.35						
MgHCO3+	1.965e-04	1.222e-04	-3.707	-3.913	-0.207	
6.21						
MgCO3	9.553e-05	1.116e-04	-4.020	-3.952	0.068	-
17.02						
MgOH+	3.916e-05	2.735e-05	-4.407	-4.563	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.141e-01	-0.354	-0.503	-0.149	
0.11						

NaSO4-	2.132e-03	1.426e-03	-2.671	-2.846	-0.175
20.79					
NaCO3-	1.252e-04	9.270e-05	-3.903	-4.033	-0.130
4.25					
NaHCO3	1.071e-04	1.251e-04	-3.970	-3.903	0.068
1.80					
NaOH	1.305e-16	1.525e-16	-15.884	-15.817	0.068
(0)					
O(0)	0.000e+00				
O2	0.000e+00	0.000e+00	-57.989	-57.921	0.068
31.43					
S(-2)	1.225e-26				
HS-	1.202e-26	7.229e-27	-25.920	-26.141	-0.221
21.92					
H2S	2.269e-28	2.651e-28	-27.644	-27.577	0.068
37.20					
S-2	2.107e-30	3.916e-31	-29.676	-30.407	-0.731
(0)					
S(6)	1.100e-02				
SO4-2	4.714e-03	8.233e-04	-2.327	-3.084	-0.758
19.24					
MgSO4	3.022e-03	3.531e-03	-2.520	-2.452	0.068
6.35					
NaSO4-	2.132e-03	1.426e-03	-2.671	-2.846	-0.175
20.79					
CaSO4	1.131e-03	1.322e-03	-2.946	-2.879	0.068
8.01					
HSO4-	9.871e-10	7.310e-10	-9.006	-9.136	-0.130
41.79					
CaHSO4+	9.673e-11	7.164e-11	-10.014	-10.145	-0.130
(0)					

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

Phase	SI**	log IAP	log K(314 K, 11 atm)	
Anhydrite	-0.72	-5.18	-4.46	CaSO4
Aragonite	1.22	-7.22	-8.45	CaCO3
Calcite	1.35	-7.22	-8.58	CaCO3
CH4(g)	-26.08	-29.01	-2.92	CH4
CO2(g)	-3.37	-5.01	-1.64	CO2
Dolomite	3.16	-14.26	-17.42	CaMg(CO3)2
Gypsum	-0.60	-5.19	-4.59	CaSO4:2H2O
H2(g)	-11.66	-14.79	-3.13	H2
H2O(g)	-1.12	-0.01	1.11	H2O
H2S(g)	-26.37	-34.34	-7.96	H2S
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-54.93	-57.92	-2.99	O2
Sulfur	-20.53	-16.01	4.52	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.153 Seconds.

Input file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\P&T
pairs\T=47, 61 atm.pqi

Output file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\P&T
pairs\T=47, 61 atm.pqi

Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 47
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
61

Beginning of initial solution calculations.

Initial solution 1.

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

--

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

--

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 47°C)	=	75719
Density (g/cm^3)	=	1.01348
Volume (L)	=	1.02050
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.745e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.893e-03
Total CO2 (mol/kg)	=	1.893e-03
Temperature (°C)	=	47.00
Electrical balance (eq)	=	1.460e-02
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23
Iterations	=	7
Total H	=	1.110140e+02
Total O	=	5.555596e+01

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

--

mole V Species cm^3/mol	Molality	Activity	Log		Gamma	
			Molality	Activity		
OH-	1.187e-05	7.101e-06	-4.925	-5.149	-0.223	-
2.13 H+	8.439e-09	6.310e-09	-8.074	-8.200	-0.126	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.21 C(4)	1.893e-03					
HCO3-	1.042e-03	6.942e-04	-2.982	-3.159	-0.176	
27.83 MgHCO3+	1.840e-04	1.138e-04	-3.735	-3.944	-0.209	
6.26 NaCO3-	1.587e-04	1.170e-04	-3.800	-3.932	-0.132	
4.41 CaCO3	1.446e-04	1.689e-04	-3.840	-3.772	0.067	-
14.54						

CaHCO3+	1.277e-04	8.727e-05	-3.894	-4.059	-0.166	
10.60						
MgCO3	9.954e-05	1.163e-04	-4.002	-3.935	0.067	-
17.10						
NaHCO3	9.300e-05	1.086e-04	-4.032	-3.964	0.067	
1.80						
CO3-2	3.635e-05	7.157e-06	-4.439	-5.145	-0.706	-
1.89						
CO2	7.408e-06	8.653e-06	-5.130	-5.063	0.067	
35.51						
(CO2) 2	2.233e-12	2.608e-12	-11.651	-11.584	0.067	
71.02						
Ca	3.500e-02					
Ca+2	3.362e-02	7.935e-03	-1.473	-2.100	-0.627	-
16.42						
CaSO4	1.103e-03	1.289e-03	-2.957	-2.890	0.067	
8.13						
CaCO3	1.446e-04	1.689e-04	-3.840	-3.772	0.067	-
14.54						
CaHCO3+	1.277e-04	8.727e-05	-3.894	-4.059	-0.166	
10.60						
CaOH+	2.776e-07	2.048e-07	-6.557	-6.689	-0.132	
(0)						
CaHSO4+	1.044e-10	7.701e-11	-9.981	-10.113	-0.132	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.545e-01	-0.243	-0.450	-0.208	
19.10						
H (0)	3.935e-28					
H2	1.968e-28	2.298e-28	-27.706	-27.639	0.067	
28.59						
Mg	4.800e-02					
Mg+2	4.442e-02	1.214e-02	-1.352	-1.916	-0.563	-
21.00						
MgSO4	3.236e-03	3.780e-03	-2.490	-2.423	0.067	
6.47						
MgHCO3+	1.840e-04	1.138e-04	-3.735	-3.944	-0.209	
6.26						
MgCO3	9.954e-05	1.163e-04	-4.002	-3.935	0.067	-
17.10						
MgOH+	6.265e-05	4.361e-05	-4.203	-4.360	-0.157	
(0)						
Na	4.450e-01					
Na+	4.427e-01	3.125e-01	-0.354	-0.505	-0.151	
0.24						
NaSO4-	2.097e-03	1.397e-03	-2.678	-2.855	-0.176	
20.60						
NaCO3-	1.587e-04	1.170e-04	-3.800	-3.932	-0.132	
4.41						
NaHCO3	9.300e-05	1.086e-04	-4.032	-3.964	0.067	
1.80						
NaOH	1.900e-16	2.219e-16	-15.721	-15.654	0.067	
(0)						
O (0)	5.325e-31					
O2	2.663e-31	3.110e-31	-30.575	-30.507	0.067	
31.77						
S (6)	1.100e-02					

SO4-2	4.564e-03	7.833e-04	-2.341	-3.106	-0.765
19.68					
MgSO4	3.236e-03	3.780e-03	-2.490	-2.423	0.067
6.47					
NaSO4-	2.097e-03	1.397e-03	-2.678	-2.855	-0.176
20.60					
CaSO4	1.103e-03	1.289e-03	-2.957	-2.890	0.067
8.13					
HSO4-	1.094e-09	8.073e-10	-8.961	-9.093	-0.132
42.03					
CaHSO4+	1.044e-10	7.701e-11	-9.981	-10.113	-0.132
(0)					

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

--

Phase	SI**	log IAP	log K(320 K,	1 atm)
Anhydrite	-0.67	-5.21	-4.54	CaSO4
Aragonite	1.26	-7.25	-8.51	CaCO3
Calcite	1.39	-7.25	-8.64	CaCO3
CO2 (g)	-3.38	-5.06	-1.69	CO2
Dolomite	3.26	-14.31	-17.57	CaMg (CO3) 2
Gypsum	-0.61	-5.22	-4.61	CaSO4:2H2O
H2 (g)	-24.50	-27.64	-3.13	H2
H2O (g)	-0.99	-0.01	0.98	H2O
Halite	-2.54	-0.96	1.59	NaCl
O2 (g)	-27.49	-30.51	-3.02	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.

Using pressure 1.

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

--

Elements	Molality	Moles
C	1.893e-03	1.893e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

pH = 8.180 Charge balance


```

pe = 8.085 Adjusted to redox
equilibrium
  Specific Conductance (µS/cm, 47°C) = 75666
    Density (g/cm³) = 1.01600
      Volume (L) = 1.01796
        Activity of water = 0.981
          Ionic strength (mol/kgw) = 6.745e-01
            Mass of water (kg) = 1.000e+00
              Total alkalinity (eq/kg) = 2.400e-03
                Total CO2 (mol/kg) = 1.893e-03
                  Temperature (°C) = 47.00
                    Pressure (atm) = 61.00
                      Electrical balance (eq) = 1.460e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
Iterations = 10
Total H = 1.110140e+02
Total O = 5.555596e+01

```

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

mole V Species cm ³ /mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	1.185e-05	7.099e-06	-4.926	-5.149	-0.223	-
2.19 H+	8.835e-09	6.611e-09	-8.054	-8.180	-0.126	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16 C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-113.753	-113.685	0.067	
37.16 C(4)	1.893e-03					
HCO3-	1.034e-03	6.897e-04	-2.985	-3.161	-0.176	
27.89 MgHCO3+	1.839e-04	1.139e-04	-3.735	-3.943	-0.208	
6.43 NaCO3-	1.588e-04	1.173e-04	-3.799	-3.931	-0.132	
4.92 CaCO3	1.463e-04	1.709e-04	-3.835	-3.767	0.067	-
14.14 CaHCO3+	1.278e-04	8.739e-05	-3.894	-4.059	-0.165	
10.72 MgCO3	1.003e-04	1.171e-04	-3.999	-3.931	0.067	-
16.66 NaHCO3	9.832e-05	1.148e-04	-4.007	-3.940	0.067	
1.80 CO3-2	3.667e-05	7.256e-06	-4.436	-5.139	-0.704	-
1.40 CO2	7.273e-06	8.495e-06	-5.138	-5.071	0.067	
35.45 (CO2)2	2.152e-12	2.513e-12	-11.667	-11.600	0.067	
70.89 Ca	3.500e-02					

Ca+2	3.362e-02	7.976e-03	-1.473	-2.098	-0.625	-
16.02						
CaSO4	1.104e-03	1.290e-03	-2.957	-2.890	0.067	
8.27						
CaCO3	1.463e-04	1.709e-04	-3.835	-3.767	0.067	-
14.14						
CaHCO3+	1.278e-04	8.739e-05	-3.894	-4.059	-0.165	
10.72						
CaOH+	2.673e-07	1.974e-07	-6.573	-6.705	-0.132	
(0)						
CaHSO4+	1.114e-10	8.228e-11	-9.953	-10.085	-0.132	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.550e-01	-0.243	-0.450	-0.207	
19.11						
H(0)	2.740e-36					
H2	1.370e-36	1.600e-36	-35.863	-35.796	0.067	
28.56						
Mg	4.800e-02					
Mg+2	4.444e-02	1.221e-02	-1.352	-1.913	-0.561	-
20.55						
MgSO4	3.217e-03	3.758e-03	-2.492	-2.425	0.067	
6.61						
MgHCO3+	1.839e-04	1.139e-04	-3.735	-3.943	-0.208	
6.43						
MgCO3	1.003e-04	1.171e-04	-3.999	-3.931	0.067	-
16.66						
MgOH+	5.973e-05	4.162e-05	-4.224	-4.381	-0.157	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.129e-01	-0.354	-0.505	-0.151	
0.43						
NaSO4-	2.110e-03	1.407e-03	-2.676	-2.852	-0.176	
20.22						
NaCO3-	1.588e-04	1.173e-04	-3.799	-3.931	-0.132	
4.92						
NaHCO3	9.832e-05	1.148e-04	-4.007	-3.940	0.067	
1.80						
NaOH	1.894e-16	2.213e-16	-15.723	-15.655	0.067	
(0)						
O(0)	9.742e-15					
O2	4.871e-15	5.689e-15	-14.312	-14.245	0.067	
31.64						
S(-2)	0.000e+00					
HS-	0.000e+00	0.000e+00	-110.597	-110.819	-0.223	
22.03						
H2S	0.000e+00	0.000e+00	-112.370	-112.303	0.067	
37.12						
S-2	0.000e+00	0.000e+00	-114.190	-114.926	-0.736	
(0)						
S(6)	1.100e-02					
SO4-2	4.569e-03	7.884e-04	-2.340	-3.103	-0.763	
19.46						
MgSO4	3.217e-03	3.758e-03	-2.492	-2.425	0.067	
6.61						
NaSO4-	2.110e-03	1.407e-03	-2.676	-2.852	-0.176	
20.22						

CaSO4	1.104e-03	1.290e-03	-2.957	-2.890	0.067
8.27					
HSO4-	1.095e-09	8.089e-10	-8.960	-9.092	-0.132
41.85					
CaHSO4+	1.114e-10	8.228e-11	-9.953	-10.085	-0.132
(0)					

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

Phase	SI**	log IAP	log K(320 K, 61 atm)	
Anhydrite	-0.71	-5.20	-4.50	CaSO4
Aragonite	1.22	-7.24	-8.46	CaCO3
Calcite	1.35	-7.24	-8.58	CaCO3
CH4(g)	-110.70	-113.69	-2.98	CH4
CO2(g)	-3.35	-5.07	-1.72	CO2
Dolomite	3.17	-14.29	-17.46	CaMg(CO3)2
Gypsum	-0.64	-5.22	-4.58	CaSO4:2H2O
H2(g)	-32.63	-35.80	-3.16	H2
H2O(g)	-0.97	-0.01	0.96	H2O
H2S(g)	-111.03	-119.00	-7.97	H2S
Halite	-2.55	-0.95	1.59	NaCl
O2(g)	-11.20	-14.24	-3.05	O2
Sulfur	-84.14	-79.77	4.37	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

 Reading input data for simulation 2.

 End of Run after 0.156 Seconds.

Input file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
 C, P variable\P = 15psi.pqi
 Output file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
 C, P variable\P = 15psi.pqi
 Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
 15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
1

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67832
Density (g/cm^3)	=	1.01647
Volume (L)	=	1.01750
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.753e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.989e-03

Total CO2 (mol/kg) = 1.989e-03
 Temperature (°C) = 40.00
 Electrical balance (eq) = 1.460e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
 Iterations = 7
 Total H = 1.110141e+02
 Total O = 5.555622e+01

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

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm ³ /mol						
OH-	7.568e-06	4.553e-06	-5.121	-5.342	-0.221	-
2.19						
H+	8.413e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(4)	1.989e-03					
HCO3-	1.160e-03	7.764e-04	-2.935	-3.110	-0.174	
27.66						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
CO3-2	3.684e-05	7.386e-06	-4.434	-5.132	-0.698	-
1.66						
CO2	8.476e-06	9.902e-06	-5.072	-5.004	0.068	
35.16						
(CO2)2	2.427e-12	2.835e-12	-11.615	-11.547	0.068	
70.32						
Ca	3.500e-02					
Ca+2	3.360e-02	8.086e-03	-1.474	-2.092	-0.619	-
16.46						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
CaOH+	2.817e-07	2.087e-07	-6.550	-6.681	-0.130	
(0)						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						
Cl	5.720e-01					

Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	4.185e-28					
H2	2.093e-28	2.445e-28	-27.679	-27.612	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.244e-02	-1.350	-1.905	-0.555	-
20.81						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
MgOH+	3.650e-05	2.551e-05	-4.438	-4.593	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.142e-01	-0.354	-0.503	-0.149	
0.05						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
NaOH	1.225e-16	1.431e-16	-15.912	-15.844	0.068	
(0)						
O(0)	4.672e-33					
O2	2.336e-33	2.729e-33	-32.632	-32.564	0.068	
31.40						
S(6)	1.100e-02					
SO4-2	4.738e-03	8.290e-04	-2.324	-3.081	-0.757	
19.21						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
HSO4-	9.700e-10	7.187e-10	-9.013	-9.143	-0.130	
41.78						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.72	-5.17	-4.45	CaSO4
Aragonite	1.22	-7.22	-8.45	CaCO3
Calcite	1.36	-7.22	-8.58	CaCO3
CO2(g)	-3.38	-5.00	-1.63	CO2
Dolomite	3.16	-14.26	-17.42	CaMg(CO3)2
Gypsum	-0.59	-5.19	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O

Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-29.58	-32.56	-2.98	O2

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
 Using pressure 1.

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

Elements	Molality	Moles
C	1.989e-03	1.989e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

	pH =	8.200	Charge balance
	pe =	8.786	Adjusted to redox
equilibrium			
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67832	
Density (g/cm^3)	=	1.01647	
Volume (L)	=	1.01750	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.753e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	2.400e-03	
Total CO2 (mol/kg)	=	1.989e-03	
Temperature (°C)	=	40.00	
Electrical balance (eq)	=	1.460e-02	
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23	
Iterations	=	9	
Total H	=	1.110141e+02	
Total O	=	5.555622e+01	

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

			Log	Log	Log
mole V					
Species	Molality	Activity	Molality	Activity	Gamma
cm^3/mol					

OH-	7.568e-06	4.553e-06	-5.121	-5.342	-0.221	-
2.19						
H+	8.413e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-118.533	-118.465	0.068	
36.62						
C(4)	1.989e-03					
HCO3-	1.160e-03	7.764e-04	-2.935	-3.110	-0.174	
27.65						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
CO3-2	3.684e-05	7.386e-06	-4.434	-5.132	-0.698	-
1.66						
CO2	8.476e-06	9.902e-06	-5.072	-5.004	0.068	
35.16						
(CO2)2	2.427e-12	2.835e-12	-11.615	-11.547	0.068	
70.32						
Ca	3.500e-02					
Ca+2	3.360e-02	8.086e-03	-1.474	-2.092	-0.619	-
16.46						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
CaOH+	2.817e-07	2.087e-07	-6.550	-6.681	-0.130	
(0)						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	1.122e-37					
H2	5.612e-38	6.556e-38	-37.251	-37.183	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.244e-02	-1.350	-1.905	-0.555	-
20.81						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						

MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
MgOH+	3.650e-05	2.551e-05	-4.438	-4.593	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.142e-01	-0.354	-0.503	-0.149	
0.05						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
NaOH	1.225e-16	1.431e-16	-15.912	-15.844	0.068	
(0)						
O(0)	6.497e-14					
O2	3.249e-14	3.795e-14	-13.488	-13.421	0.068	
31.40						
S(-2)	0.000e+00					
HS-	0.000e+00	0.000e+00	-115.376	-115.596	-0.221	
21.90						
H2S	0.000e+00	0.000e+00	-117.091	-117.024	0.068	
37.21						
S-2	0.000e+00	0.000e+00	-119.160	-119.890	-0.730	
(0)						
S(6)	1.100e-02					
SO4-2	4.738e-03	8.290e-04	-2.324	-3.081	-0.757	
19.21						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
HSO4-	9.700e-10	7.187e-10	-9.013	-9.143	-0.130	
41.78						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.72	-5.17	-4.45	CaSO4
Aragonite	1.22	-7.22	-8.45	CaCO3
Calcite	1.36	-7.22	-8.58	CaCO3
CH4(g)	-115.55	-118.47	-2.91	CH4
CO2(g)	-3.38	-5.00	-1.63	CO2
Dolomite	3.16	-14.26	-17.42	CaMg(CO3)2
Gypsum	-0.59	-5.19	-4.60	CaSO4:2H2O
H2(g)	-34.06	-37.18	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
H2S(g)	-115.83	-123.80	-7.96	H2S
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-10.44	-13.42	-2.98	O2
Sulfur	-87.60	-83.05	4.55	S

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.162 Seconds.

Input file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
C, P variable\P = 50 psi.pqi
Output file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
C, P variable\P = 50 psi.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg

REACTION_PRESSURE 1

3

 Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

	pH	=	8.200
	pe	=	4.000
Specific Conductance	($\mu\text{S}/\text{cm}$, 40°C)	=	67832
	Density (g/cm^3)	=	1.01647
	Volume (L)	=	1.01750
	Activity of water	=	0.981
	Ionic strength (mol/kgw)	=	6.753e-01
	Mass of water (kg)	=	1.000e+00
	Total carbon (mol/kg)	=	1.989e-03
	Total CO2 (mol/kg)	=	1.989e-03
	Temperature (°C)	=	40.00
	Electrical balance (eq)	=	1.460e-02
Percent error,	$100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23
	Iterations	=	7
	Total H	=	1.110141e+02
	Total O	=	5.555622e+01

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

mole V Species cm^3/mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	7.568e-06	4.553e-06	-5.121	-5.342	-0.221	-
2.19 H+	8.413e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16 C(4)	1.989e-03					
HCO3-	1.160e-03	7.764e-04	-2.935	-3.110	-0.174	
27.66						

MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
CO3-2	3.684e-05	7.386e-06	-4.434	-5.132	-0.698	-
1.66						
CO2	8.476e-06	9.902e-06	-5.072	-5.004	0.068	
35.16						
(CO2) 2	2.427e-12	2.835e-12	-11.615	-11.547	0.068	
70.32						
Ca	3.500e-02					
Ca+2	3.360e-02	8.086e-03	-1.474	-2.092	-0.619	-
16.46						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
CaOH+	2.817e-07	2.087e-07	-6.550	-6.681	-0.130	
(0)						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	4.185e-28					
H2	2.093e-28	2.445e-28	-27.679	-27.612	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.244e-02	-1.350	-1.905	-0.555	-
20.81						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
MgOH+	3.650e-05	2.551e-05	-4.438	-4.593	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.142e-01	-0.354	-0.503	-0.149	
0.05						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						

NaOH	1.225e-16	1.431e-16	-15.912	-15.844	0.068
(0)					
O(0)	4.672e-33				
O2	2.336e-33	2.729e-33	-32.632	-32.564	0.068
31.40					
S(6)	1.100e-02				
SO4-2	4.738e-03	8.290e-04	-2.324	-3.081	-0.757
19.21					
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068
6.30					
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174
20.90					
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068
7.96					
HSO4-	9.700e-10	7.187e-10	-9.013	-9.143	-0.130
41.78					
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.72	-5.17	-4.45	CaSO4
Aragonite	1.22	-7.22	-8.45	CaCO3
Calcite	1.36	-7.22	-8.58	CaCO3
CO2(g)	-3.38	-5.00	-1.63	CO2
Dolomite	3.16	-14.26	-17.42	CaMg(CO3)2
Gypsum	-0.59	-5.19	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-29.58	-32.56	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
C	1.989e-03	1.989e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01

S 1.100e-02 1.100e-02

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

pH = 8.199 Charge balance
 pe = 8.786 Adjusted to redox
 equilibrium
 Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C) = 67832
 Density (g/cm^3) = 1.01656
 Volume (L) = 1.01741
 Activity of water = 0.981
 Ionic strength (mol/kgw) = 6.753e-01
 Mass of water (kg) = 1.000e+00
 Total alkalinity (eq/kg) = 2.400e-03
 Total CO2 (mol/kg) = 1.989e-03
 Temperature (°C) = 40.00
 Pressure (atm) = 3.00
 Electrical balance (eq) = 1.460e-02
 Percent error, $100 \cdot (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = 1.23
 Iterations = 9
 Total H = 1.110141e+02
 Total O = 5.555622e+01

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

mole V Species cm^3/mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	7.567e-06	4.553e-06	-5.121	-5.342	-0.221	-
2.19						
H+	8.426e-09	6.320e-09	-8.074	-8.199	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-118.527	-118.460	0.068	
36.62						
C(4)	1.989e-03					
HCO3-	1.160e-03	7.763e-04	-2.936	-3.110	-0.174	
27.66						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.17						
CaHCO3+	1.381e-04	9.475e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.449e-04	-3.907	-3.839	0.068	-
14.54						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.12						
NaHCO3	1.085e-04	1.268e-04	-3.964	-3.897	0.068	
1.80						
MgCO3	9.453e-05	1.104e-04	-4.024	-3.957	0.068	-
17.08						

CO3-2	3.685e-05	7.389e-06	-4.434	-5.131	-0.698	-
1.64						
CO2	8.472e-06	9.897e-06	-5.072	-5.004	0.068	
35.16						
(CO2)2	2.424e-12	2.832e-12	-11.615	-11.548	0.068	
70.32						
Ca	3.500e-02					
Ca+2	3.360e-02	8.087e-03	-1.474	-2.092	-0.619	-
16.45						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.97						
CaHCO3+	1.381e-04	9.475e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.449e-04	-3.907	-3.839	0.068	-
14.54						
CaOH+	2.813e-07	2.084e-07	-6.551	-6.681	-0.130	
(0)						
CaHSO4+	9.452e-11	7.003e-11	-10.024	-10.155	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	1.124e-37					
H2	5.622e-38	6.568e-38	-37.250	-37.183	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.244e-02	-1.350	-1.905	-0.555	-
20.80						
MgSO4	2.989e-03	3.492e-03	-2.524	-2.457	0.068	
6.31						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.17						
MgCO3	9.453e-05	1.104e-04	-4.024	-3.957	0.068	-
17.08						
MgOH+	3.644e-05	2.547e-05	-4.438	-4.594	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.143e-01	-0.354	-0.503	-0.149	
0.06						
NaSO4-	2.136e-03	1.430e-03	-2.670	-2.845	-0.174	
20.88						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.12						
NaHCO3	1.085e-04	1.268e-04	-3.964	-3.897	0.068	
1.80						
NaOH	1.225e-16	1.431e-16	-15.912	-15.845	0.068	
(0)						
O(0)	6.446e-14					
O2	3.223e-14	3.765e-14	-13.492	-13.424	0.068	
31.39						
S(-2)	0.000e+00					
HS-	0.000e+00	0.000e+00	-115.370	-115.591	-0.221	
21.90						
H2S	0.000e+00	0.000e+00	-117.086	-117.018	0.068	
37.21						
S-2	0.000e+00	0.000e+00	-119.154	-119.884	-0.730	
(0)						

S(6)	1.100e-02					
SO4-2	4.739e-03	8.292e-04	-2.324	-3.081	-0.757	
19.20						
MgSO4	2.989e-03	3.492e-03	-2.524	-2.457	0.068	
6.31						
NaSO4-	2.136e-03	1.430e-03	-2.670	-2.845	-0.174	
20.88						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.97						
HSO4-	9.702e-10	7.188e-10	-9.013	-9.143	-0.130	
41.78						
CaHSO4+	9.452e-11	7.003e-11	-10.024	-10.155	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	3 atm)
Anhydrite	-0.72	-5.17	-4.45	CaSO4
Aragonite	1.22	-7.22	-8.44	CaCO3
Calcite	1.35	-7.22	-8.58	CaCO3
CH4(g)	-115.55	-118.46	-2.91	CH4
CO2(g)	-3.38	-5.00	-1.63	CO2
Dolomite	3.16	-14.26	-17.42	CaMg(CO3)2
Gypsum	-0.59	-5.19	-4.60	CaSO4:2H2O
H2(g)	-34.05	-37.18	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
H2S(g)	-115.83	-123.79	-7.96	H2S
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-10.44	-13.42	-2.99	O2
Sulfur	-87.60	-83.05	4.55	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.142 Seconds.

Input file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
C, P variable\P = 100 psi.pqi
Output file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
C, P variable\P = 100 psi.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
7

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH = 8.200
pe = 4.000

Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C) = 67832
 Density (g/cm^3) = 1.01647
 Volume (L) = 1.01750
 Activity of water = 0.981
 Ionic strength (mol/kgw) = $6.753\text{e-}01$
 Mass of water (kg) = $1.000\text{e+}00$
 Total carbon (mol/kg) = $1.989\text{e-}03$
 Total CO_2 (mol/kg) = $1.989\text{e-}03$
 Temperature ($^\circ\text{C}$) = 40.00
 Electrical balance (eq) = $1.460\text{e-}02$
 Percent error, $100 * (\text{Cat-}|\text{An}|) / (\text{Cat+}|\text{An}|)$ = 1.23
 Iterations = 7
 Total H = $1.110141\text{e+}02$
 Total O = $5.555622\text{e+}01$

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

--

mole V Species cm^3/mol	Molality	Activity	Log		Gamma	
			Molality	Activity		
OH-	$7.568\text{e-}06$	$4.553\text{e-}06$	-5.121	-5.342	-0.221	-
2.19 H+	$8.413\text{e-}09$	$6.310\text{e-}09$	-8.075	-8.200	-0.125	
0.00 H ₂ O	$5.551\text{e+}01$	$9.812\text{e-}01$	1.744	-0.008	0.000	
18.16 C(4)	$1.989\text{e-}03$					
HCO ₃ -	$1.160\text{e-}03$	$7.764\text{e-}04$	-2.935	-3.110	-0.174	
27.66 MgHCO ₃ +	$1.985\text{e-}04$	$1.235\text{e-}04$	-3.702	-3.908	-0.206	
6.16 CaHCO ₃ +	$1.381\text{e-}04$	$9.474\text{e-}05$	-3.860	-4.023	-0.164	
10.44 CaCO ₃	$1.240\text{e-}04$	$1.448\text{e-}04$	-3.907	-3.839	0.068	-
14.56 NaCO ₃ -	$1.199\text{e-}04$	$8.882\text{e-}05$	-3.921	-4.052	-0.130	
4.11 NaHCO ₃	$1.083\text{e-}04$	$1.265\text{e-}04$	-3.965	-3.898	0.068	
1.80 MgCO ₃	$9.451\text{e-}05$	$1.104\text{e-}04$	-4.025	-3.957	0.068	-
17.10 CO ₃ -2	$3.684\text{e-}05$	$7.386\text{e-}06$	-4.434	-5.132	-0.698	-
1.66 CO ₂	$8.476\text{e-}06$	$9.902\text{e-}06$	-5.072	-5.004	0.068	
35.16 (CO ₂) ₂	$2.427\text{e-}12$	$2.835\text{e-}12$	-11.615	-11.547	0.068	
70.32 Ca	$3.500\text{e-}02$					
Ca+2	$3.360\text{e-}02$	$8.086\text{e-}03$	-1.474	-2.092	-0.619	-
16.46 CaSO ₄	$1.136\text{e-}03$	$1.327\text{e-}03$	-2.945	-2.877	0.068	
7.96 CaHCO ₃ +	$1.381\text{e-}04$	$9.474\text{e-}05$	-3.860	-4.023	-0.164	
10.44						

CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
CaOH+	2.817e-07	2.087e-07	-6.550	-6.681	-0.130	
(0)						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	4.185e-28					
H2	2.093e-28	2.445e-28	-27.679	-27.612	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.244e-02	-1.350	-1.905	-0.555	-
20.81						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
MgOH+	3.650e-05	2.551e-05	-4.438	-4.593	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.142e-01	-0.354	-0.503	-0.149	
0.05						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
NaOH	1.225e-16	1.431e-16	-15.912	-15.844	0.068	
(0)						
O(0)	4.672e-33					
O2	2.336e-33	2.729e-33	-32.632	-32.564	0.068	
31.40						
S(6)	1.100e-02					
SO4-2	4.738e-03	8.290e-04	-2.324	-3.081	-0.757	
19.21						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
HSO4-	9.700e-10	7.187e-10	-9.013	-9.143	-0.130	
41.78						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K, 1 atm)
Anhydrite	-0.72	-5.17	-4.45 CaSO4

Aragonite	1.22	-7.22	-8.45	CaCO3
Calcite	1.36	-7.22	-8.58	CaCO3
CO2(g)	-3.38	-5.00	-1.63	CO2
Dolomite	3.16	-14.26	-17.42	CaMg(CO3)2
Gypsum	-0.59	-5.19	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-29.58	-32.56	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
 Using pressure 1.

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

Elements	Molality	Moles
C	1.989e-03	1.989e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

	pH =	8.198	Charge balance
	pe =	8.786	Adjusted to redox
equilibrium			
	Specific Conductance (µS/cm, 40°C)	=	67832
	Density (g/cm³)	=	1.01673
	Volume (L)	=	1.01724
	Activity of water	=	0.981
	Ionic strength (mol/kgw)	=	6.753e-01
	Mass of water (kg)	=	1.000e+00
	Total alkalinity (eq/kg)	=	2.400e-03
	Total CO2 (mol/kg)	=	1.989e-03
	Temperature (°C)	=	40.00
	Pressure (atm)	=	7.00
	Electrical balance (eq)	=	1.460e-02
Percent error, 100*(Cat- An)/(Cat+ An)		=	1.23
	Iterations	=	9
	Total H	=	1.110141e+02
	Total O	=	5.555622e+01

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

--

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	7.565e-06	4.552e-06	-5.121	-5.342	-0.221	-
2.19						
H+	8.454e-09	6.342e-09	-8.073	-8.198	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.15						
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-118.523	-118.456	0.068	
36.63						
C(4)	1.989e-03					
HCO3-	1.160e-03	7.760e-04	-2.936	-3.110	-0.174	
27.66						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.18						
CaHCO3+	1.381e-04	9.476e-05	-3.860	-4.023	-0.164	
10.45						
CaCO3	1.241e-04	1.450e-04	-3.906	-3.839	0.068	-
14.52						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.051	-0.130	
4.16						
NaHCO3	1.089e-04	1.273e-04	-3.963	-3.895	0.068	
1.80						
MgCO3	9.456e-05	1.105e-04	-4.024	-3.957	0.068	-
17.05						
CO3-2	3.686e-05	7.395e-06	-4.433	-5.131	-0.698	-
1.61						
CO2	8.464e-06	9.887e-06	-5.072	-5.005	0.068	
35.15						
(CO2)2	2.420e-12	2.827e-12	-11.616	-11.549	0.068	
70.31						
Ca	3.500e-02					
Ca+2	3.360e-02	8.090e-03	-1.474	-2.092	-0.618	-
16.42						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.98						
CaHCO3+	1.381e-04	9.476e-05	-3.860	-4.023	-0.164	
10.45						
CaCO3	1.241e-04	1.450e-04	-3.906	-3.839	0.068	-
14.52						
CaOH+	2.805e-07	2.078e-07	-6.552	-6.682	-0.130	
(0)						
CaHSO4+	9.495e-11	7.035e-11	-10.023	-10.153	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	1.124e-37					
H2	5.620e-38	6.565e-38	-37.250	-37.183	0.068	
28.59						

Mg	4.800e-02						
Mg+2	4.468e-02	1.245e-02	-1.350	-1.905	-0.555	-	
20.76							
MgSO4	2.988e-03	3.491e-03	-2.525	-2.457	0.068		
6.32							
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206		
6.18							
MgCO3	9.456e-05	1.105e-04	-4.024	-3.957	0.068	-	
17.05							
MgOH+	3.631e-05	2.538e-05	-4.440	-4.595	-0.156		
(0)							
Na	4.450e-01						
Na+	4.426e-01	3.143e-01	-0.354	-0.503	-0.149		
0.07							
NaSO4-	2.137e-03	1.430e-03	-2.670	-2.845	-0.174		
20.86							
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.051	-0.130		
4.16							
NaHCO3	1.089e-04	1.273e-04	-3.963	-3.895	0.068		
1.80							
NaOH	1.224e-16	1.430e-16	-15.912	-15.845	0.068		
(0)							
O(0)	6.401e-14						
O2	3.200e-14	3.739e-14	-13.495	-13.427	0.068		
31.39							
S(-2)	0.000e+00						
HS-	0.000e+00	0.000e+00	-115.367	-115.588	-0.221		
21.90							
H2S	0.000e+00	0.000e+00	-117.082	-117.014	0.068		
37.20							
S-2	0.000e+00	0.000e+00	-119.151	-119.881	-0.730		
(0)							
S(6)	1.100e-02						
SO4-2	4.739e-03	8.296e-04	-2.324	-3.081	-0.757		
19.18							
MgSO4	2.988e-03	3.491e-03	-2.525	-2.457	0.068		
6.32							
NaSO4-	2.137e-03	1.430e-03	-2.670	-2.845	-0.174		
20.86							
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068		
7.98							
HSO4-	9.704e-10	7.191e-10	-9.013	-9.143	-0.130		
41.76							
CaHSO4+	9.495e-11	7.035e-11	-10.023	-10.153	-0.130		
(0)							

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

Phase	SI**	log IAP	log K(313 K,	7 atm)
Anhydrite	-0.73	-5.17	-4.45	CaSO4
Aragonite	1.22	-7.22	-8.44	CaCO3
Calcite	1.35	-7.22	-8.57	CaCO3
CH4 (g)	-115.54	-118.46	-2.92	CH4
CO2 (g)	-3.38	-5.00	-1.63	CO2
Dolomite	3.15	-14.26	-17.41	CaMg (CO3) 2

Gypsum	-0.60	-5.19	-4.59	CaSO4:2H2O
H2 (g)	-34.05	-37.18	-3.13	H2
H2O (g)	-1.14	-0.01	1.14	H2O
H2S (g)	-115.82	-123.79	-7.96	H2S
Halite	-2.53	-0.95	1.58	NaCl
O2 (g)	-10.44	-13.43	-2.99	O2
Sulfur	-87.59	-83.05	4.54	S

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.143 Seconds.

Input file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
C, P variable\P = 200 psii.pqi
Output file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
C, P variable\P = 200 psii.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat
SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1

```

Ca      35
Mg      48
Na     445
S(6)    11
Alkalinity 2.4 as HCO3-
Cl      572
water   1 # kg
REACTION_PRESSURE 1
14

```

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

```

pH = 8.200
pe = 4.000
Specific Conductance (µS/cm, 40°C) = 67832
Density (g/cm³) = 1.01647
Volume (L) = 1.01750
Activity of water = 0.981
Ionic strength (mol/kgw) = 6.753e-01
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 1.989e-03
Total CO2 (mol/kg) = 1.989e-03
Temperature (°C) = 40.00
Electrical balance (eq) = 1.460e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
Iterations = 7
Total H = 1.110141e+02
Total O = 5.555622e+01

```

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

mole V Species cm ³ /mol	Molality	Activity	Log	Log	Log
			Molality	Activity	Gamma
OH- 2.19	7.568e-06	4.553e-06	-5.121	-5.342	-0.221

H+	8.413e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(4)	1.989e-03					
HCO3-	1.160e-03	7.764e-04	-2.935	-3.110	-0.174	
27.66						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
CO3-2	3.684e-05	7.386e-06	-4.434	-5.132	-0.698	-
1.66						
CO2	8.476e-06	9.902e-06	-5.072	-5.004	0.068	
35.16						
(CO2)2	2.427e-12	2.835e-12	-11.615	-11.547	0.068	
70.32						
Ca	3.500e-02					
Ca+2	3.360e-02	8.086e-03	-1.474	-2.092	-0.619	-
16.46						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
CaOH+	2.817e-07	2.087e-07	-6.550	-6.681	-0.130	
(0)						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	4.185e-28					
H2	2.093e-28	2.445e-28	-27.679	-27.612	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.244e-02	-1.350	-1.905	-0.555	-
20.81						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
MgOH+	3.650e-05	2.551e-05	-4.438	-4.593	-0.156	
(0)						
Na	4.450e-01					

Na+	4.426e-01	3.142e-01	-0.354	-0.503	-0.149
0.05					
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174
20.90					
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130
4.11					
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068
1.80					
NaOH	1.225e-16	1.431e-16	-15.912	-15.844	0.068
(0)					
O(0)	4.672e-33				
O2	2.336e-33	2.729e-33	-32.632	-32.564	0.068
31.40					
S(6)	1.100e-02				
SO4-2	4.738e-03	8.290e-04	-2.324	-3.081	-0.757
19.21					
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068
6.30					
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174
20.90					
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068
7.96					
HSO4-	9.700e-10	7.187e-10	-9.013	-9.143	-0.130
41.78					
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.72	-5.17	-4.45	CaSO4
Aragonite	1.22	-7.22	-8.45	CaCO3
Calcite	1.36	-7.22	-8.58	CaCO3
CO2(g)	-3.38	-5.00	-1.63	CO2
Dolomite	3.16	-14.26	-17.42	CaMg(CO3)2
Gypsum	-0.59	-5.19	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-29.58	-32.56	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
C	1.989e-03	1.989e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	8.195	Charge balance
	pe =	8.787	Adjusted to redox
equilibrium			
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67833	
Density (g/cm^3)	=	1.01702	
Volume (L)	=	1.01695	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.753e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	2.400e-03	
Total CO2 (mol/kg)	=	1.989e-03	
Temperature (°C)	=	40.00	
Pressure (atm)	=	14.00	
Electrical balance (eq)	=	1.460e-02	
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23	
Iterations	=	9	
Total H	=	1.110141e+02	
Total O	=	5.555622e+01	

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	Gamma
			Molality	Activity		
OH-	7.561e-06	4.550e-06	-5.121	-5.342	-0.221	-
2.19						
H+	8.503e-09	6.379e-09	-8.070	-8.195	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.15						
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-118.513	-118.445	0.068	
36.63						
C(4)	1.989e-03					
HCO3-	1.159e-03	7.755e-04	-2.936	-3.110	-0.174	
27.67						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.20						
CaHCO3+	1.381e-04	9.477e-05	-3.860	-4.023	-0.164	
10.47						

CaCO3	1.242e-04	1.451e-04	-3.906	-3.838	0.068	-
14.47						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.051	-0.130	
4.22						
NaHCO3	1.097e-04	1.281e-04	-3.960	-3.892	0.068	
1.80						
MgCO3	9.462e-05	1.105e-04	-4.024	-3.957	0.068	-
17.00						
CO3-2	3.690e-05	7.405e-06	-4.433	-5.130	-0.697	-
1.55						
CO2	8.449e-06	9.870e-06	-5.073	-5.006	0.068	
35.15						
(CO2) 2	2.411e-12	2.817e-12	-11.618	-11.550	0.068	
70.30						
Ca	3.500e-02					
Ca+2	3.360e-02	8.095e-03	-1.474	-2.092	-0.618	-
16.37						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
8.00						
CaHCO3+	1.381e-04	9.477e-05	-3.860	-4.023	-0.164	
10.47						
CaCO3	1.242e-04	1.451e-04	-3.906	-3.838	0.068	-
14.47						
CaOH+	2.791e-07	2.068e-07	-6.554	-6.684	-0.130	
(0)						
CaHSO4+	9.571e-11	7.092e-11	-10.019	-10.149	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.567e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	1.125e-37					
H2	5.627e-38	6.573e-38	-37.250	-37.182	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.246e-02	-1.350	-1.905	-0.555	-
20.71						
MgSO4	2.986e-03	3.488e-03	-2.525	-2.457	0.068	
6.34						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.20						
MgCO3	9.462e-05	1.105e-04	-4.024	-3.957	0.068	-
17.00						
MgOH+	3.609e-05	2.523e-05	-4.443	-4.598	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.143e-01	-0.354	-0.503	-0.149	
0.09						
NaSO4-	2.138e-03	1.431e-03	-2.670	-2.844	-0.174	
20.81						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.051	-0.130	
4.22						
NaHCO3	1.097e-04	1.281e-04	-3.960	-3.892	0.068	
1.80						
NaOH	1.223e-16	1.429e-16	-15.913	-15.845	0.068	
(0)						
O(0)	6.294e-14					

O2	3.147e-14	3.677e-14	-13.502	-13.435	0.068
31.37					
S(-2)	0.000e+00				
HS-	0.000e+00	0.000e+00	-115.357	-115.578	-0.221
21.90					
H2S	0.000e+00	0.000e+00	-117.071	-117.004	0.068
37.19					
S-2	0.000e+00	0.000e+00	-119.141	-119.871	-0.730
(0)					
S(6)	1.100e-02				
SO4-2	4.740e-03	8.303e-04	-2.324	-3.081	-0.757
19.15					
MgSO4	2.986e-03	3.488e-03	-2.525	-2.457	0.068
6.34					
NaSO4-	2.138e-03	1.431e-03	-2.670	-2.844	-0.174
20.81					
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068
8.00					
HSO4-	9.709e-10	7.195e-10	-9.013	-9.143	-0.130
41.74					
CaHSO4+	9.571e-11	7.092e-11	-10.019	-10.149	-0.130
(0)					

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

Phase	SI**	log IAP	log K(313 K, 14 atm)	
Anhydrite	-0.73	-5.17	-4.44	CaSO4
Aragonite	1.21	-7.22	-8.43	CaCO3
Calcite	1.35	-7.22	-8.57	CaCO3
CH4(g)	-115.53	-118.45	-2.92	CH4
CO2(g)	-3.37	-5.01	-1.63	CO2
Dolomite	3.14	-14.26	-17.40	CaMg(CO3)2
Gypsum	-0.60	-5.19	-4.59	CaSO4:2H2O
H2(g)	-34.05	-37.18	-3.13	H2
H2O(g)	-1.14	-0.01	1.13	H2O
H2S(g)	-115.81	-123.77	-7.97	H2S
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-10.44	-13.43	-2.99	O2
Sulfur	-87.58	-83.04	4.54	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.144 Seconds.

Input file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
C, P variable\P = 400 psi.pqi
Output file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
C, P variable\P = 400 psi.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
27

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01

Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

--

	pH	=	8.200
	pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)		=	67832
Density (g/cm^3)		=	1.01647
Volume (L)		=	1.01750
Activity of water		=	0.981
Ionic strength (mol/kgw)		=	6.753e-01
Mass of water (kg)		=	1.000e+00
Total carbon (mol/kg)		=	1.989e-03
Total CO2 (mol/kg)		=	1.989e-03
Temperature (°C)		=	40.00
Electrical balance (eq)		=	1.460e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$		=	1.23
	Iterations	=	7
	Total H	=	1.110141e+02
	Total O	=	5.555622e+01

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	7.568e-06	4.553e-06	-5.121	-5.342	-0.221	-
2.19						
H+	8.413e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(4)	1.989e-03					
HCO3-	1.160e-03	7.764e-04	-2.935	-3.110	-0.174	
27.66						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
CO3-2	3.684e-05	7.386e-06	-4.434	-5.132	-0.698	-
1.66						
CO2	8.476e-06	9.902e-06	-5.072	-5.004	0.068	
35.16						

(CO2)2	2.427e-12	2.835e-12	-11.615	-11.547	0.068	
70.32						
Ca	3.500e-02					
Ca+2	3.360e-02	8.086e-03	-1.474	-2.092	-0.619	-
16.46						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
CaOH+	2.817e-07	2.087e-07	-6.550	-6.681	-0.130	
(0)						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	4.185e-28					
H2	2.093e-28	2.445e-28	-27.679	-27.612	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.244e-02	-1.350	-1.905	-0.555	-
20.81						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
MgOH+	3.650e-05	2.551e-05	-4.438	-4.593	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.142e-01	-0.354	-0.503	-0.149	
0.05						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
NaOH	1.225e-16	1.431e-16	-15.912	-15.844	0.068	
(0)						
O(0)	4.672e-33					
O2	2.336e-33	2.729e-33	-32.632	-32.564	0.068	
31.40						
S(6)	1.100e-02					
SO4-2	4.738e-03	8.290e-04	-2.324	-3.081	-0.757	
19.21						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
HSO4-	9.700e-10	7.187e-10	-9.013	-9.143	-0.130	
41.78						

CaHSO4+ 9.430e-11 6.987e-11 -10.025 -10.156 -0.130
 (0)

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

--

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.72	-5.17	-4.45	CaSO4
Aragonite	1.22	-7.22	-8.45	CaCO3
Calcite	1.36	-7.22	-8.58	CaCO3
CO2(g)	-3.38	-5.00	-1.63	CO2
Dolomite	3.16	-14.26	-17.42	CaMg(CO3)2
Gypsum	-0.59	-5.19	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-29.58	-32.56	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
 Using pressure 1.

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

--

Elements	Molality	Moles
C	1.989e-03	1.989e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

	pH =	8.191	Charge balance
	pe =	8.788	Adjusted to redox
equilibrium			
	Specific Conductance (µS/cm, 40°C)	=	67833
	Density (g/cm³)	=	1.01757
	Volume (L)	=	1.01640
	Activity of water	=	0.981
	Ionic strength (mol/kgw)	=	6.754e-01
	Mass of water (kg)	=	1.000e+00
	Total alkalinity (eq/kg)	=	2.400e-03
	Total CO2 (mol/kg)	=	1.989e-03

Temperature (°C) = 40.00
 Pressure (atm) = 27.00
 Electrical balance (eq) = 1.460e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
 Iterations = 9
 Total H = 1.110141e+02
 Total O = 5.555622e+01

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

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	7.553e-06	4.547e-06	-5.122	-5.342	-0.220	-
2.19						
H+	8.595e-09	6.449e-09	-8.066	-8.191	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.14						
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-118.496	-118.429	0.068	
36.65						
C(4)	1.989e-03					
HCO3-	1.157e-03	7.745e-04	-2.937	-3.111	-0.174	
27.68						
MgHCO3+	1.986e-04	1.236e-04	-3.702	-3.908	-0.206	
6.24						
CaHCO3+	1.381e-04	9.481e-05	-3.860	-4.023	-0.163	
10.49						
CaCO3	1.245e-04	1.454e-04	-3.905	-3.837	0.068	-
14.38						
NaCO3-	1.198e-04	8.882e-05	-3.921	-4.051	-0.130	
4.34						
NaHCO3	1.110e-04	1.297e-04	-3.955	-3.887	0.068	
1.80						
MgCO3	9.472e-05	1.107e-04	-4.024	-3.956	0.068	-
16.90						
CO3-2	3.695e-05	7.424e-06	-4.432	-5.129	-0.697	-
1.45						
CO2	8.421e-06	9.838e-06	-5.075	-5.007	0.068	
35.14						
(CO2)2	2.395e-12	2.798e-12	-11.621	-11.553	0.068	
70.28						
Ca	3.500e-02					
Ca+2	3.360e-02	8.104e-03	-1.474	-2.091	-0.618	-
16.28						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
8.03						
CaHCO3+	1.381e-04	9.481e-05	-3.860	-4.023	-0.163	
10.49						
CaCO3	1.245e-04	1.454e-04	-3.905	-3.837	0.068	-
14.38						
CaOH+	2.766e-07	2.050e-07	-6.558	-6.688	-0.130	
(0)						

CaHSO4+	9.713e-11	7.200e-11	-10.013	-10.143	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.568e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	1.126e-37					
H2	5.631e-38	6.578e-38	-37.249	-37.182	0.068	
28.58						
Mg	4.800e-02					
Mg+2	4.469e-02	1.247e-02	-1.350	-1.904	-0.554	-
20.61						
MgSO4	2.982e-03	3.484e-03	-2.525	-2.458	0.068	
6.37						
MgHCO3+	1.986e-04	1.236e-04	-3.702	-3.908	-0.206	
6.24						
MgCO3	9.472e-05	1.107e-04	-4.024	-3.956	0.068	-
16.90						
MgOH+	3.569e-05	2.495e-05	-4.447	-4.603	-0.155	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.144e-01	-0.354	-0.502	-0.149	
0.13						
NaSO4-	2.140e-03	1.432e-03	-2.670	-2.844	-0.174	
20.72						
NaCO3-	1.198e-04	8.882e-05	-3.921	-4.051	-0.130	
4.34						
NaHCO3	1.110e-04	1.297e-04	-3.955	-3.887	0.068	
1.80						
NaOH	1.221e-16	1.427e-16	-15.913	-15.846	0.068	
(0)						
O(0)	6.121e-14					
O2	3.060e-14	3.575e-14	-13.514	-13.447	0.068	
31.35						
S(-2)	0.000e+00					
HS-	0.000e+00	0.000e+00	-115.342	-115.563	-0.220	
21.90						
H2S	0.000e+00	0.000e+00	-117.054	-116.987	0.068	
37.16						
S-2	0.000e+00	0.000e+00	-119.126	-119.856	-0.729	
(0)						
S(6)	1.100e-02					
SO4-2	4.743e-03	8.316e-04	-2.324	-3.080	-0.756	
19.10						
MgSO4	2.982e-03	3.484e-03	-2.525	-2.458	0.068	
6.37						
NaSO4-	2.140e-03	1.432e-03	-2.670	-2.844	-0.174	
20.72						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
8.03						
HSO4-	9.716e-10	7.202e-10	-9.012	-9.143	-0.130	
41.71						
CaHSO4+	9.713e-11	7.200e-11	-10.013	-10.143	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K, 27 atm)	
Anhydrite	-0.74	-5.17	-4.43	CaSO4
Aragonite	1.20	-7.22	-8.42	CaCO3
Calcite	1.33	-7.22	-8.56	CaCO3
CH4(g)	-115.50	-118.43	-2.93	CH4
CO2(g)	-3.37	-5.01	-1.64	CO2
Dolomite	3.12	-14.25	-17.38	CaMg(CO3)2
Gypsum	-0.61	-5.19	-4.58	CaSO4:2H2O
H2(g)	-34.04	-37.18	-3.14	H2
H2O(g)	-1.14	-0.01	1.13	H2O
H2S(g)	-115.78	-123.75	-7.97	H2S
Halite	-2.54	-0.95	1.58	NaCl
O2(g)	-10.45	-13.45	-3.00	O2
Sulfur	-87.56	-83.03	4.53	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.134 Seconds.

Input file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
C, P variable\P = 550 psi.pqi
Output file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
C, P variable\P = 550 psi.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
37

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67832
Density (g/cm^3)	=	1.01647
Volume (L)	=	1.01750
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.753e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.989e-03
Total CO2 (mol/kg)	=	1.989e-03
Temperature (°C)	=	40.00
Electrical balance (eq)	=	1.460e-02
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23
Iterations	=	7
Total H	=	1.110141e+02
Total O	=	5.555622e+01

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

--

mole V Species cm ³ /mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	7.568e-06	4.553e-06	-5.121	-5.342	-0.221	-
2.19						
H+	8.413e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(4)	1.989e-03					
HCO3-	1.160e-03	7.764e-04	-2.935	-3.110	-0.174	
27.66						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
CO3-2	3.684e-05	7.386e-06	-4.434	-5.132	-0.698	-
1.66						
CO2	8.476e-06	9.902e-06	-5.072	-5.004	0.068	
35.16						
(CO2)2	2.427e-12	2.835e-12	-11.615	-11.547	0.068	
70.32						
Ca	3.500e-02					
Ca+2	3.360e-02	8.086e-03	-1.474	-2.092	-0.619	-
16.46						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
CaOH+	2.817e-07	2.087e-07	-6.550	-6.681	-0.130	
(0)						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	4.185e-28					
H2	2.093e-28	2.445e-28	-27.679	-27.612	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.244e-02	-1.350	-1.905	-0.555	-
20.81						

MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
MgOH+	3.650e-05	2.551e-05	-4.438	-4.593	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.142e-01	-0.354	-0.503	-0.149	
0.05						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
NaOH	1.225e-16	1.431e-16	-15.912	-15.844	0.068	
(0)						
O(0)	4.672e-33					
O2	2.336e-33	2.729e-33	-32.632	-32.564	0.068	
31.40						
S(6)	1.100e-02					
SO4-2	4.738e-03	8.290e-04	-2.324	-3.081	-0.757	
19.21						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
HSO4-	9.700e-10	7.187e-10	-9.013	-9.143	-0.130	
41.78						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.72	-5.17	-4.45	CaSO4
Aragonite	1.22	-7.22	-8.45	CaCO3
Calcite	1.36	-7.22	-8.58	CaCO3
CO2(g)	-3.38	-5.00	-1.63	CO2
Dolomite	3.16	-14.26	-17.42	CaMg(CO3)2
Gypsum	-0.59	-5.19	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-29.58	-32.56	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.

Using pressure 1.

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

Elements	Molality	Moles
C	1.989e-03	1.989e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

	pH =	8.187	Charge balance
	pe =	8.789	Adjusted to redox
equilibrium			
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67833	
Density (g/cm^3)	=	1.01799	
Volume (L)	=	1.01598	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.754e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	2.400e-03	
Total CO2 (mol/kg)	=	1.989e-03	
Temperature (°C)	=	40.00	
Pressure (atm)	=	37.00	
Electrical balance (eq)	=	1.460e-02	
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23	
Iterations	=	9	
Total H	=	1.110141e+02	
Total O	=	5.555622e+01	

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

mole V Species cm^3/mol	Molality	Activity	Log		Log	
			Molality	Activity	Gamma	
OH-	7.548e-06	4.545e-06	-5.122	-5.342	-0.220	-
2.19						
H+	8.666e-09	6.503e-09	-8.062	-8.187	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.13						
C(-4)	0.000e+00					

CH4	0.000e+00	0.000e+00	-118.483	-118.415	0.068	
36.66						
C(4)	1.989e-03					
HCO3-	1.156e-03	7.738e-04	-2.937	-3.111	-0.174	
27.69						
MgHCO3+	1.986e-04	1.236e-04	-3.702	-3.908	-0.206	
6.27						
CaHCO3+	1.381e-04	9.484e-05	-3.860	-4.023	-0.163	
10.51						
CaCO3	1.247e-04	1.456e-04	-3.904	-3.837	0.068	-
14.31						
NaCO3-	1.198e-04	8.882e-05	-3.922	-4.051	-0.130	
4.42						
NaHCO3	1.121e-04	1.309e-04	-3.951	-3.883	0.068	
1.80						
MgCO3	9.480e-05	1.108e-04	-4.023	-3.956	0.068	-
16.83						
CO3-2	3.699e-05	7.438e-06	-4.432	-5.129	-0.697	-
1.37						
CO2	8.400e-06	9.813e-06	-5.076	-5.008	0.068	
35.13						
(CO2)2	2.383e-12	2.784e-12	-11.623	-11.555	0.068	
70.26						
Ca	3.500e-02					
Ca+2	3.360e-02	8.111e-03	-1.474	-2.091	-0.617	-
16.22						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
8.06						
CaHCO3+	1.381e-04	9.484e-05	-3.860	-4.023	-0.163	
10.51						
CaCO3	1.247e-04	1.456e-04	-3.904	-3.837	0.068	-
14.31						
CaOH+	2.747e-07	2.036e-07	-6.561	-6.691	-0.130	
(0)						
CaHSO4+	9.824e-11	7.283e-11	-10.008	-10.138	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.569e-01	-0.243	-0.447	-0.205	
19.08						
H(0)	1.127e-37					
H2	5.637e-38	6.585e-38	-37.249	-37.181	0.068	
28.58						
Mg	4.800e-02					
Mg+2	4.469e-02	1.248e-02	-1.350	-1.904	-0.554	-
20.54						
MgSO4	2.979e-03	3.480e-03	-2.526	-2.458	0.068	
6.40						
MgHCO3+	1.986e-04	1.236e-04	-3.702	-3.908	-0.206	
6.27						
MgCO3	9.480e-05	1.108e-04	-4.023	-3.956	0.068	-
16.83						
MgOH+	3.539e-05	2.475e-05	-4.451	-4.606	-0.155	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.145e-01	-0.354	-0.502	-0.148	
0.16						

NaSO4-	2.141e-03	1.434e-03	-2.669	-2.844	-0.174
20.66					
NaCO3-	1.198e-04	8.882e-05	-3.922	-4.051	-0.130
4.42					
NaHCO3	1.121e-04	1.309e-04	-3.951	-3.883	0.068
1.80					
NaOH	1.220e-16	1.425e-16	-15.914	-15.846	0.068
(0)					
O(0)	5.985e-14				
O2	2.993e-14	3.496e-14	-13.524	-13.456	0.068
31.33					
S(-2)	0.000e+00				
HS-	0.000e+00	0.000e+00	-115.330	-115.550	-0.220
21.90					
H2S	0.000e+00	0.000e+00	-117.041	-116.973	0.068
37.15					
S-2	0.000e+00	0.000e+00	-119.114	-119.843	-0.729
(0)					
S(6)	1.100e-02				
SO4-2	4.744e-03	8.325e-04	-2.324	-3.080	-0.756
19.06					
MgSO4	2.979e-03	3.480e-03	-2.526	-2.458	0.068
6.40					
NaSO4-	2.141e-03	1.434e-03	-2.669	-2.844	-0.174
20.66					
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068
8.06					
HSO4-	9.722e-10	7.207e-10	-9.012	-9.142	-0.130
41.68					
CaHSO4+	9.824e-11	7.283e-11	-10.008	-10.138	-0.130
(0)					

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

Phase	SI**	log IAP	log K(313 K, 37 atm)	
Anhydrite	-0.75	-5.17	-4.43	CaSO4
Aragonite	1.20	-7.22	-8.41	CaCO3
Calcite	1.33	-7.22	-8.55	CaCO3
CH4(g)	-115.48	-118.42	-2.93	CH4
CO2(g)	-3.36	-5.01	-1.65	CO2
Dolomite	3.11	-14.25	-17.36	CaMg(CO3)2
Gypsum	-0.61	-5.19	-4.58	CaSO4:2H2O
H2(g)	-34.04	-37.18	-3.15	H2
H2O(g)	-1.14	-0.01	1.13	H2O
H2S(g)	-115.76	-123.74	-7.98	H2S
Halite	-2.54	-0.95	1.59	NaCl
O2(g)	-10.45	-13.46	-3.00	O2
Sulfur	-87.55	-83.02	4.53	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.223 Seconds.

Input file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
C, P variable\P = 600 psi.pqi
Output file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
C, P variable\P = 600 psi.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
41

Beginning of initial solution calculations.

Initial solution 1.

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

--

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

--

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67832
Density (g/cm^3)	=	1.01647
Volume (L)	=	1.01750
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.753e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.989e-03
Total CO2 (mol/kg)	=	1.989e-03
Temperature (°C)	=	40.00
Electrical balance (eq)	=	1.460e-02
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23
Iterations	=	7
Total H	=	1.110141e+02
Total O	=	5.555622e+01

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

--

mole V Species cm^3/mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	7.568e-06	4.553e-06	-5.121	-5.342	-0.221	-
2.19 H+	8.413e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16 C(4)	1.989e-03					
HCO3-	1.160e-03	7.764e-04	-2.935	-3.110	-0.174	
27.66 MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16 CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44 CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						

NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
CO3-2	3.684e-05	7.386e-06	-4.434	-5.132	-0.698	-
1.66						
CO2	8.476e-06	9.902e-06	-5.072	-5.004	0.068	
35.16						
(CO2) 2	2.427e-12	2.835e-12	-11.615	-11.547	0.068	
70.32						
Ca	3.500e-02					
Ca+2	3.360e-02	8.086e-03	-1.474	-2.092	-0.619	-
16.46						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
CaOH+	2.817e-07	2.087e-07	-6.550	-6.681	-0.130	
(0)						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H (0)	4.185e-28					
H2	2.093e-28	2.445e-28	-27.679	-27.612	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.244e-02	-1.350	-1.905	-0.555	-
20.81						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
MgOH+	3.650e-05	2.551e-05	-4.438	-4.593	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.142e-01	-0.354	-0.503	-0.149	
0.05						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
NaOH	1.225e-16	1.431e-16	-15.912	-15.844	0.068	
(0)						
O (0)	4.672e-33					
O2	2.336e-33	2.729e-33	-32.632	-32.564	0.068	
31.40						
S (6)	1.100e-02					

SO4-2	4.738e-03	8.290e-04	-2.324	-3.081	-0.757
19.21					
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068
6.30					
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174
20.90					
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068
7.96					
HSO4-	9.700e-10	7.187e-10	-9.013	-9.143	-0.130
41.78					
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130
(0)					

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

--

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.72	-5.17	-4.45	CaSO4
Aragonite	1.22	-7.22	-8.45	CaCO3
Calcite	1.36	-7.22	-8.58	CaCO3
CO2 (g)	-3.38	-5.00	-1.63	CO2
Dolomite	3.16	-14.26	-17.42	CaMg (CO3) 2
Gypsum	-0.59	-5.19	-4.60	CaSO4:2H2O
H2 (g)	-24.48	-27.61	-3.13	H2
H2O (g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2 (g)	-29.58	-32.56	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

--

Elements	Molality	Moles
C	1.989e-03	1.989e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

--

pH = 8.185 Charge balance

```

pe = 8.790 Adjusted to redox
equilibrium
  Specific Conductance (µS/cm, 40°C) = 67833
    Density (g/cm³) = 1.01816
      Volume (L) = 1.01581
        Activity of water = 0.981
          Ionic strength (mol/kgw) = 6.754e-01
            Mass of water (kg) = 1.000e+00
              Total alkalinity (eq/kg) = 2.400e-03
                Total CO2 (mol/kg) = 1.989e-03
                  Temperature (°C) = 40.00
                    Pressure (atm) = 41.00
                      Electrical balance (eq) = 1.460e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
Iterations = 9
Total H = 1.110141e+02
Total O = 5.555622e+01

```

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

mole V Species cm ³ /mol	Molality	Activity	Log	Log	Log	
			Molality	Activity	Gamma	
OH-	7.546e-06	4.544e-06	-5.122	-5.343	-0.220	-
2.19 H+	8.695e-09	6.525e-09	-8.061	-8.185	-0.125	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.13 C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-118.478	-118.411	0.068	
36.66 C(4)	1.989e-03					
HCO3-	1.155e-03	7.735e-04	-2.937	-3.112	-0.174	
27.69 MgHCO3+	1.986e-04	1.236e-04	-3.702	-3.908	-0.206	
6.28 CaHCO3+	1.382e-04	9.485e-05	-3.860	-4.023	-0.163	
10.52 CaCO3	1.247e-04	1.457e-04	-3.904	-3.836	0.068	-
14.28 NaCO3-	1.198e-04	8.882e-05	-3.922	-4.052	-0.130	
4.46 NaHCO3	1.125e-04	1.314e-04	-3.949	-3.881	0.068	
1.80 MgCO3	9.484e-05	1.108e-04	-4.023	-3.955	0.068	-
16.80 CO3-2	3.701e-05	7.444e-06	-4.432	-5.128	-0.696	-
1.33 CO2	8.392e-06	9.803e-06	-5.076	-5.009	0.068	
35.13 (CO2)2	2.379e-12	2.779e-12	-11.624	-11.556	0.068	
70.25 Ca	3.500e-02					

Ca+2	3.360e-02	8.113e-03	-1.474	-2.091	-0.617	-
16.19						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
8.07						
CaHCO3+	1.382e-04	9.485e-05	-3.860	-4.023	-0.163	
10.52						
CaCO3	1.247e-04	1.457e-04	-3.904	-3.836	0.068	-
14.28						
CaOH+	2.739e-07	2.031e-07	-6.562	-6.692	-0.130	
(0)						
CaHSO4+	9.869e-11	7.317e-11	-10.006	-10.136	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.569e-01	-0.243	-0.447	-0.205	
19.08						
H(0)	1.127e-37					
H2	5.636e-38	6.584e-38	-37.249	-37.182	0.068	
28.57						
Mg	4.800e-02					
Mg+2	4.469e-02	1.249e-02	-1.350	-1.904	-0.554	-
20.51						
MgSO4	2.978e-03	3.479e-03	-2.526	-2.459	0.068	
6.41						
MgHCO3+	1.986e-04	1.236e-04	-3.702	-3.908	-0.206	
6.28						
MgCO3	9.484e-05	1.108e-04	-4.023	-3.955	0.068	-
16.80						
MgOH+	3.527e-05	2.466e-05	-4.453	-4.608	-0.155	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.145e-01	-0.354	-0.502	-0.148	
0.17						
NaSO4-	2.142e-03	1.434e-03	-2.669	-2.843	-0.174	
20.63						
NaCO3-	1.198e-04	8.882e-05	-3.922	-4.052	-0.130	
4.46						
NaHCO3	1.125e-04	1.314e-04	-3.949	-3.881	0.068	
1.80						
NaOH	1.220e-16	1.425e-16	-15.914	-15.846	0.068	
(0)						
O(0)	5.939e-14					
O2	2.969e-14	3.469e-14	-13.527	-13.460	0.068	
31.32						
S(-2)	0.000e+00					
HS-	0.000e+00	0.000e+00	-115.326	-115.546	-0.220	
21.90						
H2S	0.000e+00	0.000e+00	-117.037	-116.969	0.068	
37.14						
S-2	0.000e+00	0.000e+00	-119.110	-119.839	-0.729	
(0)						
S(6)	1.100e-02					
SO4-2	4.745e-03	8.329e-04	-2.324	-3.079	-0.756	
19.04						
MgSO4	2.978e-03	3.479e-03	-2.526	-2.459	0.068	
6.41						
NaSO4-	2.142e-03	1.434e-03	-2.669	-2.843	-0.174	
20.63						

CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068
8.07					
HSO4-	9.724e-10	7.209e-10	-9.012	-9.142	-0.130
41.67					
CaHSO4+	9.869e-11	7.317e-11	-10.006	-10.136	-0.130
(0)					

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

Phase	SI**	log IAP	log K(313 K, 41 atm)	
Anhydrite	-0.75	-5.17	-4.42	CaSO4
Aragonite	1.19	-7.22	-8.41	CaCO3
Calcite	1.32	-7.22	-8.54	CaCO3
CH4(g)	-115.47	-118.41	-2.94	CH4
CO2(g)	-3.36	-5.01	-1.65	CO2
Dolomite	3.10	-14.25	-17.35	CaMg(CO3)2
Gypsum	-0.61	-5.19	-4.57	CaSO4:2H2O
H2(g)	-34.03	-37.18	-3.15	H2
H2O(g)	-1.13	-0.01	1.13	H2O
H2S(g)	-115.75	-123.73	-7.98	H2S
Halite	-2.54	-0.95	1.59	NaCl
O2(g)	-10.45	-13.46	-3.01	O2
Sulfur	-87.54	-83.02	4.52	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.136 Seconds.

Input file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
C, P variable\P = 800 psi.pqi
Output file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
C, P variable\P = 800 psi.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg
REACTION_PRESSURE 1
54

Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

pH	=	8.200
pe	=	4.000
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67832
Density (g/cm^3)	=	1.01647
Volume (L)	=	1.01750
Activity of water	=	0.981
Ionic strength (mol/kgw)	=	6.753e-01
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.989e-03

Total CO2 (mol/kg) = 1.989e-03
 Temperature (°C) = 40.00
 Electrical balance (eq) = 1.460e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 1.23
 Iterations = 7
 Total H = 1.110141e+02
 Total O = 5.555622e+01

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

mole V			Log	Log	Log	
Species	Molality	Activity	Molality	Activity	Gamma	
cm ³ /mol						
OH-	7.568e-06	4.553e-06	-5.121	-5.342	-0.221	-
2.19						
H+	8.413e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16						
C(4)	1.989e-03					
HCO3-	1.160e-03	7.764e-04	-2.935	-3.110	-0.174	
27.66						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
CO3-2	3.684e-05	7.386e-06	-4.434	-5.132	-0.698	-
1.66						
CO2	8.476e-06	9.902e-06	-5.072	-5.004	0.068	
35.16						
(CO2)2	2.427e-12	2.835e-12	-11.615	-11.547	0.068	
70.32						
Ca	3.500e-02					
Ca+2	3.360e-02	8.086e-03	-1.474	-2.092	-0.619	-
16.46						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
CaOH+	2.817e-07	2.087e-07	-6.550	-6.681	-0.130	
(0)						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						
Cl	5.720e-01					

Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	4.185e-28					
H2	2.093e-28	2.445e-28	-27.679	-27.612	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.244e-02	-1.350	-1.905	-0.555	-
20.81						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
MgOH+	3.650e-05	2.551e-05	-4.438	-4.593	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.142e-01	-0.354	-0.503	-0.149	
0.05						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
NaOH	1.225e-16	1.431e-16	-15.912	-15.844	0.068	
(0)						
O(0)	4.672e-33					
O2	2.336e-33	2.729e-33	-32.632	-32.564	0.068	
31.40						
S(6)	1.100e-02					
SO4-2	4.738e-03	8.290e-04	-2.324	-3.081	-0.757	
19.21						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
HSO4-	9.700e-10	7.187e-10	-9.013	-9.143	-0.130	
41.78						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.72	-5.17	-4.45	CaSO4
Aragonite	1.22	-7.22	-8.45	CaCO3
Calcite	1.36	-7.22	-8.58	CaCO3
CO2(g)	-3.38	-5.00	-1.63	CO2
Dolomite	3.16	-14.26	-17.42	CaMg(CO3)2
Gypsum	-0.59	-5.19	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O

Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-29.58	-32.56	-2.98	O2

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
 Using pressure 1.

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

Elements	Molality	Moles
C	1.989e-03	1.989e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S	1.100e-02	1.100e-02

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

	pH =	8.181	Charge balance
	pe =	8.791	Adjusted to redox
equilibrium			
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67833	
Density (g/cm^3)	=	1.01871	
Volume (L)	=	1.01526	
Activity of water	=	0.981	
Ionic strength (mol/kgw)	=	6.754e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	2.400e-03	
Total CO2 (mol/kg)	=	1.989e-03	
Temperature (°C)	=	40.00	
Pressure (atm)	=	54.00	
Electrical balance (eq)	=	1.460e-02	
Percent error, $100 * (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23	
Iterations	=	9	
Total H	=	1.110141e+02	
Total O	=	5.555622e+01	

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

			Log	Log	Log	
mole V	Species	Molality	Activity	Molality	Activity	Gamma
		cm^3/mol				

OH-	7.539e-06	4.542e-06	-5.123	-5.343	-0.220	-
2.19						
H+	8.788e-09	6.596e-09	-8.056	-8.181	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.12						
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-118.461	-118.393	0.068	
36.67						
C(4)	1.989e-03					
HCO3-	1.153e-03	7.725e-04	-2.938	-3.112	-0.174	
27.70						
MgHCO3+	1.986e-04	1.237e-04	-3.702	-3.908	-0.206	
6.32						
CaHCO3+	1.382e-04	9.489e-05	-3.860	-4.023	-0.163	
10.55						
CaCO3	1.250e-04	1.460e-04	-3.903	-3.836	0.068	-
14.19						
NaCO3-	1.198e-04	8.880e-05	-3.922	-4.052	-0.130	
4.57						
NaHCO3	1.139e-04	1.330e-04	-3.944	-3.876	0.068	
1.80						
MgCO3	9.495e-05	1.109e-04	-4.023	-3.955	0.068	-
16.71						
CO3-2	3.705e-05	7.461e-06	-4.431	-5.127	-0.696	-
1.23						
CO2	8.364e-06	9.771e-06	-5.078	-5.010	0.068	
35.11						
(CO2)2	2.363e-12	2.761e-12	-11.627	-11.559	0.068	
70.23						
Ca	3.500e-02					
Ca+2	3.360e-02	8.122e-03	-1.474	-2.090	-0.617	-
16.10						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
8.10						
CaHCO3+	1.382e-04	9.489e-05	-3.860	-4.023	-0.163	
10.55						
CaCO3	1.250e-04	1.460e-04	-3.903	-3.836	0.068	-
14.19						
CaOH+	2.715e-07	2.013e-07	-6.566	-6.696	-0.130	
(0)						
CaHSO4+	1.002e-10	7.427e-11	-9.999	-10.129	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.570e-01	-0.243	-0.447	-0.205	
19.09						
H(0)	1.128e-37					
H2	5.642e-38	6.591e-38	-37.249	-37.181	0.068	
28.57						
Mg	4.800e-02					
Mg+2	4.470e-02	1.250e-02	-1.350	-1.903	-0.553	-
20.41						
MgSO4	2.974e-03	3.474e-03	-2.527	-2.459	0.068	
6.44						
MgHCO3+	1.986e-04	1.237e-04	-3.702	-3.908	-0.206	
6.32						

MgCO3	9.495e-05	1.109e-04	-4.023	-3.955	0.068	-
16.71						
MgOH+	3.488e-05	2.440e-05	-4.457	-4.613	-0.155	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.146e-01	-0.354	-0.502	-0.148	
0.21						
NaSO4-	2.144e-03	1.436e-03	-2.669	-2.843	-0.174	
20.55						
NaCO3-	1.198e-04	8.880e-05	-3.922	-4.052	-0.130	
4.57						
NaHCO3	1.139e-04	1.330e-04	-3.944	-3.876	0.068	
1.80						
NaOH	1.218e-16	1.423e-16	-15.914	-15.847	0.068	
(0)						
O(0)	5.772e-14					
O2	2.886e-14	3.372e-14	-13.540	-13.472	0.068	
31.29						
S(-2)	0.000e+00					
HS-	0.000e+00	0.000e+00	-115.310	-115.530	-0.220	
21.90						
H2S	0.000e+00	0.000e+00	-117.019	-116.952	0.068	
37.12						
S-2	0.000e+00	0.000e+00	-119.095	-119.823	-0.728	
(0)						
S(6)	1.100e-02					
SO4-2	4.747e-03	8.342e-04	-2.324	-3.079	-0.755	
18.99						
MgSO4	2.974e-03	3.474e-03	-2.527	-2.459	0.068	
6.44						
NaSO4-	2.144e-03	1.436e-03	-2.669	-2.843	-0.174	
20.55						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
8.10						
HSO4-	9.731e-10	7.215e-10	-9.012	-9.142	-0.130	
41.63						
CaHSO4+	1.002e-10	7.427e-11	-9.999	-10.129	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K, 54 atm)	
Anhydrite	-0.76	-5.17	-4.41	CaSO4
Aragonite	1.18	-7.22	-8.40	CaCO3
Calcite	1.31	-7.22	-8.53	CaCO3
CH4(g)	-115.45	-118.39	-2.94	CH4
CO2(g)	-3.35	-5.01	-1.66	CO2
Dolomite	3.08	-14.25	-17.33	CaMg(CO3)2
Gypsum	-0.62	-5.19	-4.57	CaSO4:2H2O
H2(g)	-34.03	-37.18	-3.15	H2
H2O(g)	-1.13	-0.01	1.12	H2O
H2S(g)	-115.73	-123.71	-7.98	H2S
Halite	-2.54	-0.95	1.59	NaCl
O2(g)	-10.46	-13.47	-3.01	O2
Sulfur	-87.52	-83.01	4.52	S

**For a gas, $SI = \log_{10}(\text{fugacity})$. Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.149 Seconds.

Input file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
C, P variable\P = 1000 psi.pqi
Output file: D:\KU\Thesis Writing\3) Discussion\1) Phreeqc modeling\T = 40
C, P variable\P = 1000 psi.pqi
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-
15100\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 3.6.2-
15100\database\phreeqc.dat

SOLUTION 1
temp 40
pH 8.2
pe 4
redox pe
units mmol/kgw
density 1
Ca 35
Mg 48
Na 445
S(6) 11
Alkalinity 2.4 as HCO3-
Cl 572
water 1 # kg

REACTION_PRESSURE 1

68

 Beginning of initial solution calculations.

Initial solution 1.

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

Elements	Molality	Moles
Alkalinity	2.400e-03	2.400e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01
S(6)	1.100e-02	1.100e-02

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

	pH	=	8.200
	pe	=	4.000
Specific Conductance	($\mu\text{S}/\text{cm}$, 40°C)	=	67832
	Density (g/cm^3)	=	1.01647
	Volume (L)	=	1.01750
	Activity of water	=	0.981
	Ionic strength (mol/kgw)	=	6.753e-01
	Mass of water (kg)	=	1.000e+00
	Total carbon (mol/kg)	=	1.989e-03
	Total CO2 (mol/kg)	=	1.989e-03
	Temperature (°C)	=	40.00
	Electrical balance (eq)	=	1.460e-02
Percent error,	$100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23
	Iterations	=	7
	Total H	=	1.110141e+02
	Total O	=	5.555622e+01

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

mole V Species cm^3/mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	7.568e-06	4.553e-06	-5.121	-5.342	-0.221	-
2.19 H+	8.413e-09	6.310e-09	-8.075	-8.200	-0.125	
0.00 H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.16 C(4)	1.989e-03					
HCO3-	1.160e-03	7.764e-04	-2.935	-3.110	-0.174	
27.66						

MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
CO3-2	3.684e-05	7.386e-06	-4.434	-5.132	-0.698	-
1.66						
CO2	8.476e-06	9.902e-06	-5.072	-5.004	0.068	
35.16						
(CO2) 2	2.427e-12	2.835e-12	-11.615	-11.547	0.068	
70.32						
Ca	3.500e-02					
Ca+2	3.360e-02	8.086e-03	-1.474	-2.092	-0.619	-
16.46						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
7.96						
CaHCO3+	1.381e-04	9.474e-05	-3.860	-4.023	-0.164	
10.44						
CaCO3	1.240e-04	1.448e-04	-3.907	-3.839	0.068	-
14.56						
CaOH+	2.817e-07	2.087e-07	-6.550	-6.681	-0.130	
(0)						
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.566e-01	-0.243	-0.448	-0.205	
19.08						
H(0)	4.185e-28					
H2	2.093e-28	2.445e-28	-27.679	-27.612	0.068	
28.59						
Mg	4.800e-02					
Mg+2	4.468e-02	1.244e-02	-1.350	-1.905	-0.555	-
20.81						
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068	
6.30						
MgHCO3+	1.985e-04	1.235e-04	-3.702	-3.908	-0.206	
6.16						
MgCO3	9.451e-05	1.104e-04	-4.025	-3.957	0.068	-
17.10						
MgOH+	3.650e-05	2.551e-05	-4.438	-4.593	-0.156	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.142e-01	-0.354	-0.503	-0.149	
0.05						
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174	
20.90						
NaCO3-	1.199e-04	8.882e-05	-3.921	-4.052	-0.130	
4.11						
NaHCO3	1.083e-04	1.265e-04	-3.965	-3.898	0.068	
1.80						

NaOH	1.225e-16	1.431e-16	-15.912	-15.844	0.068
(0)					
O(0)	4.672e-33				
O2	2.336e-33	2.729e-33	-32.632	-32.564	0.068
31.40					
S(6)	1.100e-02				
SO4-2	4.738e-03	8.290e-04	-2.324	-3.081	-0.757
19.21					
MgSO4	2.990e-03	3.493e-03	-2.524	-2.457	0.068
6.30					
NaSO4-	2.136e-03	1.429e-03	-2.670	-2.845	-0.174
20.90					
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068
7.96					
HSO4-	9.700e-10	7.187e-10	-9.013	-9.143	-0.130
41.78					
CaHSO4+	9.430e-11	6.987e-11	-10.025	-10.156	-0.130
(0)					

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

Phase	SI**	log IAP	log K(313 K,	1 atm)
Anhydrite	-0.72	-5.17	-4.45	CaSO4
Aragonite	1.22	-7.22	-8.45	CaCO3
Calcite	1.36	-7.22	-8.58	CaCO3
CO2(g)	-3.38	-5.00	-1.63	CO2
Dolomite	3.16	-14.26	-17.42	CaMg(CO3)2
Gypsum	-0.59	-5.19	-4.60	CaSO4:2H2O
H2(g)	-24.48	-27.61	-3.13	H2
H2O(g)	-1.15	-0.01	1.14	H2O
Halite	-2.53	-0.95	1.58	NaCl
O2(g)	-29.58	-32.56	-2.98	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
C	1.989e-03	1.989e-03
Ca	3.500e-02	3.500e-02
Cl	5.720e-01	5.720e-01
Mg	4.800e-02	4.800e-02
Na	4.450e-01	4.450e-01

S 1.100e-02 1.100e-02

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

equilibrium

	pH	=	8.176	Charge balance
	pe	=	8.793	Adjusted to redox
Specific Conductance ($\mu\text{S}/\text{cm}$, 40°C)	=	67832		
Density (g/cm^3)	=	1.01930		
Volume (L)	=	1.01468		
Activity of water	=	0.981		
Ionic strength (mol/kgw)	=	6.754e-01		
Mass of water (kg)	=	1.000e+00		
Total alkalinity (eq/kg)	=	2.400e-03		
Total CO2 (mol/kg)	=	1.989e-03		
Temperature (°C)	=	40.00		
Pressure (atm)	=	68.00		
Electrical balance (eq)	=	1.460e-02		
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.23		
Iterations	=	9		
Total H	=	1.110141e+02		
Total O	=	5.555622e+01		

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

mole V Species cm^3/mol	Molality	Activity	Log		Log Gamma	
			Molality	Activity		
OH-	7.531e-06	4.539e-06	-5.123	-5.343	-0.220	-
2.18						
H+	8.889e-09	6.674e-09	-8.051	-8.176	-0.125	
0.00						
H2O	5.551e+01	9.812e-01	1.744	-0.008	0.000	
18.10						
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-118.445	-118.377	0.068	
36.68						
C(4)	1.989e-03					
HCO3-	1.151e-03	7.714e-04	-2.939	-3.113	-0.174	
27.71						
MgHCO3+	1.986e-04	1.237e-04	-3.702	-3.908	-0.206	
6.36						
CaHCO3+	1.382e-04	9.494e-05	-3.859	-4.023	-0.163	
10.58						
CaCO3	1.253e-04	1.463e-04	-3.902	-3.835	0.068	-
14.10						
NaCO3-	1.197e-04	8.879e-05	-3.922	-4.052	-0.130	
4.69						
NaHCO3	1.154e-04	1.348e-04	-3.938	-3.870	0.068	
1.80						
MgCO3	9.506e-05	1.111e-04	-4.022	-3.954	0.068	-
16.60						

CO3-2	3.710e-05	7.479e-06	-4.431	-5.126	-0.696	-
1.12						
CO2	8.334e-06	9.736e-06	-5.079	-5.012	0.068	
35.10						
(CO2)2	2.346e-12	2.741e-12	-11.630	-11.562	0.068	
70.21						
Ca	3.500e-02					
Ca+2	3.360e-02	8.132e-03	-1.474	-2.090	-0.616	-
16.01						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
8.13						
CaHCO3+	1.382e-04	9.494e-05	-3.859	-4.023	-0.163	
10.58						
CaCO3	1.253e-04	1.463e-04	-3.902	-3.835	0.068	-
14.10						
CaOH+	2.690e-07	1.995e-07	-6.570	-6.700	-0.130	
(0)						
CaHSO4+	1.018e-10	7.547e-11	-9.992	-10.122	-0.130	
(0)						
Cl	5.720e-01					
Cl-	5.720e-01	3.572e-01	-0.243	-0.447	-0.205	
19.09						
H(0)	1.128e-37					
H2	5.640e-38	6.589e-38	-37.249	-37.181	0.068	
28.56						
Mg	4.800e-02					
Mg+2	4.470e-02	1.252e-02	-1.350	-1.903	-0.553	-
20.31						
MgSO4	2.970e-03	3.469e-03	-2.527	-2.460	0.068	
6.47						
MgHCO3+	1.986e-04	1.237e-04	-3.702	-3.908	-0.206	
6.36						
MgCO3	9.506e-05	1.111e-04	-4.022	-3.954	0.068	-
16.60						
MgOH+	3.448e-05	2.412e-05	-4.462	-4.618	-0.155	
(0)						
Na	4.450e-01					
Na+	4.426e-01	3.147e-01	-0.354	-0.502	-0.148	
0.25						
NaSO4-	2.146e-03	1.438e-03	-2.668	-2.842	-0.174	
20.46						
NaCO3-	1.197e-04	8.879e-05	-3.922	-4.052	-0.130	
4.69						
NaHCO3	1.154e-04	1.348e-04	-3.938	-3.870	0.068	
1.80						
NaOH	1.217e-16	1.421e-16	-15.915	-15.847	0.068	
(0)						
O(0)	5.613e-14					
O2	2.807e-14	3.279e-14	-13.552	-13.484	0.068	
31.27						
S(-2)	0.000e+00					
HS-	0.000e+00	0.000e+00	-115.296	-115.516	-0.220	
21.90						
H2S	0.000e+00	0.000e+00	-117.003	-116.936	0.068	
37.09						
S-2	0.000e+00	0.000e+00	-119.081	-119.809	-0.728	
(0)						

S (6)	1.100e-02					
SO4-2	4.749e-03	8.355e-04	-2.323	-3.078	-0.755	
18.93						
MgSO4	2.970e-03	3.469e-03	-2.527	-2.460	0.068	
6.47						
NaSO4-	2.146e-03	1.438e-03	-2.668	-2.842	-0.174	
20.46						
CaSO4	1.136e-03	1.327e-03	-2.945	-2.877	0.068	
8.13						
HSO4-	9.737e-10	7.222e-10	-9.012	-9.141	-0.130	
41.60						
CaHSO4+	1.018e-10	7.547e-11	-9.992	-10.122	-0.130	
(0)						

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

Phase	SI**	log IAP	log K(313 K, 68 atm)	
Anhydrite	-0.77	-5.17	-4.40	CaSO4
Aragonite	1.17	-7.22	-8.39	CaCO3
Calcite	1.30	-7.22	-8.52	CaCO3
CH4 (g)	-115.42	-118.38	-2.95	CH4
CO2 (g)	-3.35	-5.01	-1.66	CO2
Dolomite	3.06	-14.24	-17.30	CaMg (CO3) 2
Gypsum	-0.63	-5.18	-4.56	CaSO4:2H2O
H2 (g)	-34.02	-37.18	-3.16	H2
H2O (g)	-1.13	-0.01	1.12	H2O
H2S (g)	-115.70	-123.69	-7.99	H2S
Halite	-2.54	-0.95	1.59	NaCl
O2 (g)	-10.46	-13.48	-3.02	O2
Sulfur	-87.51	-83.00	4.51	S

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
 For ideal gases, phi = 1.

 End of simulation.

 Reading input data for simulation 2.

 End of Run after 0.145 Seconds.

Appendix E Python codes for calculating mol% MgCO₃ in Mg-Calcite

```
""  
Author: Zijie Gao  
Date: 11/29/2020  
Function: Calculating the Molar content of MgCO3 from XRD data  
Version : 2.0  
New function:  
1) write results into a txt document  
2) get the filename of the reading data, and output it together with the corresponded results  
""
```

```
import pandas as pd  
import xlrd  
import math  
from math import pi  
import os
```

```
def get_filename(path,filetype):  
    ""  
    Read file name  
    ""  
    name = []  
    for root,dirs,files in os.walk(path):  
        for i in files:  
            if filetype in i:  
                name.append(i.replace(filetype,""))  
    return name
```

```
def write_txt(list):  
    ""
```

```

    write results into .txt document
'''
fileObject = open('MgCO3.txt', 'a')

for ip in list:
    fileObject.writelines(str(ip))
    fileObject.write(' ')
fileObject.write("\n")

fileObject.close()

def main():
    path = 'C:\\Users\CUPGZ\Desktop\A. Research-
Experiment\\1) Before pressure\\3) DataFor Dec 19\\1) XRD\XRD_Dec 19\\3) MgCO3 Content\CalMg_ne
w'
    filetype = '.xlsx'
    name = get_filename(path, filetype)
    for word in name:
        data = xlrd.open_workbook(word + '.xlsx')
        table = data.sheets()[0]
        twotheta = table.col_values(0)
        intensity = table.col_values(1)

        # Combine two lists into one tuple
        data_tuples = list(zip(twotheta, intensity))

        # Converting list of tuples to pandas dataframe
        data_pd = pd.DataFrame(data_tuples, columns=['twotheta', 'intensity'])

        # Use two conditions to filter data and get the index

```



```

# print(data_pd[(data_pd['twotheta']>=29.7) & (data_pd['twotheta']<=29.8)])
index_list = data_pd[(data_pd['twotheta']>=29.7) & (data_pd['twotheta']<=29.8)].index.tolist()

# Sum of intensity
sum_intensity = data_pd[index_list[0]:max(index_list)+1]['intensity'].sum()
# print(sum_intensity)

# Sum of products
sum_product = 0

for i in index_list:
    product = data_pd.at[i, 'twotheta'] * data_pd.at[i, 'intensity']
    sum_product = sum_product + product

# print(sum_product)
division = sum_product/sum_intensity
# print(division)

# Calculate x
x = 1.54178/(2*math.sin((division/2)/180*pi))
# print(x)
list_result = []
list_result.append(word)

# Arvidson & Mackenzie 1999
mgco3_am = -363.96*x + 1104.5
# print(mgco3_am)
list_result.append(mgco3_am)

# Lumsden and Chimahusky 1980
mgco3_lc = 100-(333.33*x-911.99)
list_result.append(mgco3_lc)

```

```
write_txt(list_result)
```

```
print(list_result)
```

```
if __name__ == '__main__':
```

```
    main()
```