

A PDF-Based Microphysics Parameterization for Simulation of Drizzling Boundary Layer Clouds

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Abstract: Formulating the contribution of subgrid-scale (SGS) variability to microphysical processes in boundary layer and deep convective cloud parameterizations is a challenging task because of the complexity of microphysical processes and the lack of subgrid-scale information. In this study, a warm-rain microphysics parameterization that is based on a joint double-Gaussian distribution of vertical velocity, liquid water potential temperature, total water mixing ratio, and perturbation of rainwater mixing ratio is developed to simulate drizzling boundary layer clouds with a single column model (SCM). The probability distribution function (PDF) is assumed, but its parameters evolve according to equations that invoke higher-order turbulence closure. These parameters are determined from the first-, second-, and third-order moments and are then used to derive analytical expressions for autoconversion, collection, and evaporation rates. The analytical expressions show that correlation between rainwater and liquid water mixing ratios of the Gaussians enhances the collection rate whereas that between saturation deficit and rainwater mixing ratios of the Gaussians enhances the evaporation rate. Cases of drizzling shallow cumulus and stratocumulus are simulated with large-eddy simulation (LES) and SCM runs (SCM-CNTL and SCM-M): LES explicitly resolves SGS variability, SCM-CNTL parameterizes SGS variability with the PDF-based scheme, but SCM-M uses the grid-mean profiles to calculate the conversion rates of microphysical processes. SCM-CNTL can well reproduce the autoconversion, collection, and evaporation rates from LES. Comparisons between the two SCM experiments showed improvements in mean profiles of potential temperature, total water mixing ratio, liquid water, and cloud amount in the simulations considering SGS variability. A 3-week integration using the PDF-based microphysics scheme indicates that the scheme is stable for long-term simulations. [PUBLICATION ABSTRACT]

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ABSTRACT

Formulating the contribution of subgrid-scale (SGS) variability to microphysical processes in boundary layer and deep convective cloud parameterizations is a challenging task because of the complexity of microphysical processes and the lack of subgrid-scale information. In this study, a warm-rain microphysics parameterization that is based on a joint double-Gaussian distribution of vertical velocity, liquid water potential temperature, total water mixing ratio, and perturbation of rainwater mixing ratio is developed to simulate drizzling boundary layer clouds with a single column model (SCM). The probability distribution function (PDF) is assumed, but its parameters evolve according to equations that invoke higher-order turbulence closure. These parameters are determined from the first-, second-, and third-order moments and are then used to derive analytical expressions for autoconversion, collection, and evaporation rates. The analytical expressions show that correlation between rainwater and liquid water mixing ratios of the Gaussians enhances the collection rate whereas that between saturation deficit and rainwater mixing ratios of the Gaussians enhances the evaporation rate. Cases of drizzling shallow cumulus and stratocumulus are simulated with large-eddy simulation (LES) and SCM runs (SCM-CNTL and SCM-M): LES explicitly resolves SGS variability, SCM-CNTL parameterizes SGS variability with the PDF-based scheme, but SCM-M uses the grid-mean profiles to calculate the conversion rates of microphysical processes. SCM-CNTL can well reproduce the autoconversion, collection, and evaporation rates from LES. Comparisons between the two SCM experiments showed improvements in mean profiles of potential temperature, total water mixing ratio, liquid water, and cloud amount in the simulations considering SGS

variability. A 3-week integration using the PDF-based microphysics scheme indicates that the scheme is stable for long-term simulations.

1. Introduction

It is well known that variability in cloud microphysical and macrophysical properties occurs at very fine spatial and temporal scales. If subgrid-scale (SGS) variability in cloud properties is crudely represented in numerical models, potentially substantial biases in microphysical process rates can result from inadequate consideration of SGS variability (Pincus and Klein 2000; Larson et al. 2001a; Woods et al. 2002). A potential benefit for representing SGS variability properly in cloud-resolving models (CRMs) and general circulation models (GCMs) is to permit more accurate and realistic simulations of clouds and climate. For example, Bechtold et al. (1993) incorporated parts of SGS variability into a two-moment warm-rain microphysics scheme by utilizing the vertical distribution of the partial cloudiness and the environmental and cloud-scale averaged values for the thermodynamic variables instead of their grid-mean values. The formulation can greatly enhance the ability of a single column model (SCM) to simulate shallow cumulus and stratocumulus clouds. Jakob and Klein (2000) showed that a treatment of the effects of vertically varying cloud fraction in a GCM results in more reasonable estimates of local precipitation fluxes by separating grid-mean rain and snow fluxes into a cloudy and a clear-sky part.

Probability distribution functions (PDFs) are usually used to represent the SGS variability of water vapor and clouds in numerical models, which cannot be explicitly resolved by grid-scale dynamics and thermodynamics. The pioneering approach to SGS condensation by Sommeria and Deardorff (1977) and Mellor (1977) used the Gaussian PDF to represent the SGS variations of thermodynamic variables to diagnose cloud fraction and condensate mixing ratio. Bougeault (1981) compared the performance of the Gaussian PDF used in a higher-order turbulence closure model with that of a skew exponential PDF in simulating the trade wind cumulus. Although the skewness was fixed, the exponential PDF is found to be superior at parameterizing the turbulent kinetic energy (TKE) production. A variable skewness PDF using two Gaussians was proposed by Lewellen and Yoh (1993) and implemented into an SCM by Golaz et al. (2002a,b). Other forms of PDFs are also used to represent the SGS variations of water vapor and clouds, in addition to the Gaussian PDF families. For example, Smith (1990) used a symmetric triangular PDF to represent SGS variations of relative humidity to diagnose cloud fraction. A beta distribution of SGS total water mixing ratio was used in Tompkins (2002) to parameterize SGS variability of cirrus cloud decks and stratocumulus clouds.

Although the analytical solutions for liquid water mixing ratio and cloud fraction can be obtained by integrating over most of the assumed PDFs, the analytical solutions for the conversion rates of microphysical processes, such as autoconversion and collection rates, are not readily obtained because of the complexity of the PDFs. Two random sampling methods were developed to compute the SGS contributions to cloud microphysical processes: the Monte Carlo method (e.g., Jakob and Klein 2000; Pincus et al. 2003) and the Latin hypercube sampling method (Larson et al. 2005). The basic idea behind these methods is to invoke the microphysics parameterization for each sample point within each grid box at each time step. The sample points are chosen randomly from an assumed SGS distribution within each grid box. The microphysical process variables based on each sample point are then averaged properly to find the grid-mean rates. A problem related to these methods is that statistical noise is introduced at each time step, which results from an incomplete sampling of the distribution for the sake of saving computational cost. The Latin hypercube sampling method reduces variance by preventing the sample points from being clumped together within the sample space. A variance reduction method (Räisänen and Barker 2004) is also needed for the Monte Carlo method to decrease the noise.

In this study, we attempt to obtain analytical expressions for warm-rain microphysical process variables by integrating the microphysical process rates over the entire range of the PDF that describes the SGS variability. A double-Gaussian joint PDF of liquid water potential temperature ($\theta^{\text{sub } l^{\wedge}}$), total water mixing ratio ($q^{\text{sub } t^{\wedge}}$),

vertical velocity (w), and perturbation of rainwater mixing ratio ($q'^{\text{sub } r}$) will be used; it is determined from a higher-order closure scheme that predicts the first-, second-, and higher-order moments. The reason for using the double-Gaussian-based joint PDF is that it has been tested extensively for various boundary layer clouds (e.g., Larson et al. 2002) since it was introduced to cloud modeling by Lewellen and Yoh (1993). Furthermore, Golaz et al. (2002a, b) developed a higher-order turbulence closure scheme based on the double-Gaussian-based joint PDF and showed its strong abilities to simulate various types of boundary layer clouds (see also Cheng and Xu 2006, 2008).

The primary objective of this study is to propose a PDF-based microphysical formulation in the Langley Research Center (LaRC) higher-order turbulence closure scheme (Cheng et al. 2004; Cheng and Xu 2006) and to test the scheme in simulations of drizzling shallow cumulus and stratocumulus cases. The rest of the paper is organized as follows: Section 2 describes the PDF-based microphysics parameterization. Model description and experiment design are provided in section 3. Section 4 presents the results; conclusions are given in section 5.

2. Description of the microphysics parameterization

a. The assumed PDF

The family of continuous distribution functions to be used in this study is the joint double Gaussian of w , $\theta'^{\text{sub } l}$, $q'^{\text{sub } t}$ and $q'^{\text{sub } r}$. The reason for using the perturbation of the rainwater mixing ratio instead of the rainwater mixing ratio itself is that the former more likely follows the double-Gaussian PDF than the latter:

$$G(w, \theta'^{\text{sub } l}, q'^{\text{sub } t}, q'^{\text{sub } r}) = \lambda G^{\text{sub } 1}(w, \theta'^{\text{sub } l}, q'^{\text{sub } t}, q'^{\text{sub } r}) + (1 - \lambda) G^{\text{sub } 2}(w, \theta'^{\text{sub } l}, q'^{\text{sub } t}, q'^{\text{sub } r}), \quad (1)$$

with $G^{\text{sub } k}(w, \theta'^{\text{sub } l}, q'^{\text{sub } t}, q'^{\text{sub } r})$

... (2)

where λ is the relative weight of the first Gaussian, $x^{\text{sup } T^{\text{sub } k}} = [w, \theta'^{\text{sub } l}, q'^{\text{sub } t}, q'^{\text{sub } r}]^{\text{sub } k}$ is a four-component column vector representing different variables for the k th Gaussian, $\mu^{\text{sup } T^{\text{sub } k}}$ is a four-component column vector representing the means of the four variables for the k th Gaussian, and ... is an element of the covariance matrix for the k th Gaussian. In this scheme, the PDF is assumed, but the values describing the PDF (its parameters) evolve according to equations that invoke higher-order turbulence closure.

b. Rainwater autoconversion

An analytical expression for the autoconversion rate ($A^{\text{sub } c}$) can be obtained by integrating the formula of autoconversion rate over the double-Gaussian PDF. For simplicity of deriving an analytical expression, we used the Sundqvist-type formula (Sundqvist 1978):

$$A^{\text{sub } c}(q^{\text{sub } l}) = c^{\text{sub } a} [1 - \exp(-q^{\text{sup } 2^{\text{sub } l}/q^{\text{sup } 2^{\text{sub } \text{crit}}})] (q^{\text{sub } l} - q^{\text{sub } \text{crit}}), \quad (3)$$

where $q^{\text{sub } l}$ is the total liquid water mixing ratio, $c^{\text{sub } a}$ is the autoconversion time scale, and $q^{\text{sub } \text{crit}}$ is the autoconversion threshold, the values of which are given in Table 1. We define $q^{\text{sub } x}$, which is a measure of saturation, as follows:

$$q^{\text{sub } x} = q^{\text{sub } t} - q^{\text{sub } s} = a^{\text{sub } k} q^{\text{sub } t} - b^{\text{sub } k} \theta'^{\text{sub } l} + a^{\text{sub } k} (q^{\text{sub } t, k} - q^{\text{sub } s, k}), \quad (4)$$

where $q^{\text{sub } s}$ is the saturation water vapor mixing ratio at temperature T , $q^{\text{sub } s, k}$ is the mean $q^{\text{sub } s}$ at liquid-water temperature $T^{\text{sub } l, k}$ for the k th Gaussian, and $q^{\text{sub } t, k}$ is the mean q , for the k th Gaussian.

Also, $a^{\text{sub } k} = (1 + L^{\text{sup } 2^{\text{sub } v} q^{\text{sub } s, k} / R c^{\text{sub } p} T^{\text{sup } 2^{\text{sub } l, k}})^{\text{sup } -1}$ and $b^{\text{sub } k} = a^{\text{sub } k} q^{\text{sub } s, k} (L^{\text{sub } v} / R T^{\text{sup } 2^{\text{sub } l, k}} T^{\text{sub } k} / \theta^{\text{sub } k})$, where R is the constant of gas, $c^{\text{sub } p}$ is the specific heat at the constant pressure, and $L^{\text{sub } v}$ is the latent heat of vaporization at 0°C ; $q^{\text{sub } x}$ is similar to that defined by Sommeria and Deardorff (1977), Mellor (1977), and Chen (1991) except that the perturbations ($q'^{\text{sub } t}$ and $\theta'^{\text{sub } l}$) are deviated from the Gaussian means rather than the grid means (note that $q^{\text{sub } x}$ also follows the double-Gaussian distribution).

The autoconversion rate of the k th Gaussian ($A^{\text{sub } ck}$) is defined as

$$A^{\text{sub } ck} = \int_{q^{\text{sub } \text{crit}}}^{\infty} q^{\text{sup } \text{crit}} A^{\text{sub } c}(q^{\text{sub } x}) G^{\text{sub } k}(q^{\text{sub } x}) dq^{\text{sub } x}. \quad (5)$$

Here the one-component Gaussian that is identical to that used in Sommeria and Deardorff (1977) and Mellor

(1977) is used, rather than the full four-component Gaussian, because A^{c} is independent of the components related to w and q^{r} . Now A^{c} can be integrated straightforwardly as

... (6)

where ... is the standard deviation of q^{x} for the k th Gaussian, erf is the error function, and $q^{\text{l},k}$ is the mean liquid water mixing ratio of the k th Gaussian. $\alpha^{\text{k}} = (2\sigma^{\text{sk}} + q^{\text{crit}} - \sigma^{\text{sk}}q^{\text{crit}})/(\sigma^{\text{sk}}\sqrt{4\sigma^{\text{sk}} + 2q^{\text{crit}}})$, $\beta^{\text{k}} = [a^{\text{sk}}(q^{\text{t},k} - q^{\text{sl},k})^2]/(2\sigma^{\text{sk}} + q^{\text{crit}})$, and $\gamma^{\text{k}} = 1/2[1 + \text{erf}\{1/\sqrt{[(q^{\text{l},k} - q^{\text{crit}})/\sigma^{\text{sk}}]}\}]$ is the fraction of the k th Gaussian that has a liquid water mixing ratio (q^{l}) greater than q^{crit} . Thus, the fractional area of a grid cell that has q^{l} greater than q^{crit} is

$$f^{\text{cr}} = \lambda\gamma^{\text{1}} + (1 - \lambda)\gamma^{\text{2}} \quad (7)$$

The grid-mean autoconversion rate is then obtained from

$$A^{\text{c}} = \lambda A^{\text{c1}} + (1 - \lambda)A^{\text{c2}}. \quad (8)$$

c. Rainwater collection

The collection of cloud droplets by raindrops due to differences in the terminal velocity between raindrops and cloud droplets (C^{r}) can be derived based on the assumption that the Marshall and Palmer (1948) distribution is held for q^{r} :

$$C^{\text{r}}(q^{\text{l}}, q^{\text{r}}) = c^{\text{c}}q^{\text{l}}q^{\text{r}}c^{\text{1r}}. \quad (9)$$

Equation (9) is applicable for a grid box that is totally cloudy, but the formula for a partially cloudy situation needs to be derived below. See Table 1 for the values of c^{c} and c^{1r} . Because the subgrid-scale distribution of q^{t} and q^{r} is known for the assumed PDF, the collection rate for each Gaussian can be obtained from

... (10)

where ... is the grid-mean rainwater mixing ratio and $q^{\text{r},k}$ is the mean rainwater mixing ratio for the k th Gaussian, in deriving (10), a Taylor expansion is used for qr relative to the Gaussian mean. The approximate sign is introduced because of the neglect of the higher-order terms such as $q^{\text{r}2}$ and $q^{\text{r}3}$, which will become negligible in most instances provided that ... In (10),

... (11)

is the cloud fraction of the k th Gaussian. Because f^{k} is positive, a positive correlation between q^{x} and the rainwater mixing ratio enhances the collection rate. The grid-mean collection rate is then obtained from

$$C^{\text{r}} = \lambda C^{\text{r1}} + (1 - \lambda)C^{\text{r2}}. \quad (12)$$

d. Rainwater evaporation

The evaporation rate (E^{r}) can be calculated following Klemp and Wilhelmson (1978):

... (13)

where $C^{\text{e}} = c^{\text{6}} + c^{\text{7}}(pq^{\text{r}})^3$ is the ventilation factor, p is the air density, and p^{0} is a constant reference pressure (1000 hPa). See Table 1 for the values of these constants, from c^{3} to c^{7} . The evaporation rate for the k th Gaussian can be derived as follows:

... (14)

where ... and ... Notice that (4) has been used with $q^{\text{r}} = q^{\text{v}}$ because evaporation occurs in an unsaturated area. As in (10), a Taylor expansion has been used in deriving (14). One can see that a positive correlation between q^{x} and the rainwater mixing ratio tends to decrease the evaporation rate. The grid-mean evaporation rate is then obtained from

$$E^{\text{r}} = \lambda E^{\text{r1}} + (1 - \lambda)E^{\text{r2}}. \quad (15)$$

e. Closure of the microphysics parameterization

The grid-mean rainwater mixing ratio (...) is forecasted in the parent model (CRM or GCM) and the random overlap assumption is used for the precipitation falling between vertical layers. The second moment of q^{r}

is derived from

... (16)

where \dots , \dots , and L is the dissipation length scale calculated following Golaz et al. (2002a). The terms on the right-hand side of (16) are the higher-order moment, shear production, and dissipation, respectively. When the higher-order moment term is neglected and a steady state is assumed, one obtains

... (17)

Equations (8), (12), and (15) can be used to calculate the autoconversion, collection, and evaporation rates in higher-order turbulence closure (HOC) schemes. The additional unknowns introduced in these equations are $q^{\text{sub } r, k^{\wedge}}$, and $(\dots)^{\text{sub } k^{\wedge}}$, $q^{\text{sub } r, k^{\wedge}}$ can be determined from the method given in the appendix of Cheng and Xu (2006) by substituting a with $q^{\text{sub } r, k^{\wedge}}$, and

... (18)

Because the within-Gaussian correlation in the two Gaussians is further assumed to be equal as in the double-Gaussian approach (Larson et al. 2001b; Golaz et al. 2002a), that is, $r^{\text{sub } q, q^{\text{sub } r^{\wedge}, 1^{\wedge}}} = r^{\text{sub } q, q^{\text{sub } r^{\wedge}, 2^{\wedge}}}$ and $r^{\text{sub } \theta, q^{\text{sub } r^{\wedge}, 1^{\wedge}}} = r^{\text{sub } \theta, q^{\text{sub } r^{\wedge}, 2^{\wedge}}}$ one only needs to parameterize

... and (19)

... (20)

The derivation of (19) and (20) follows the same procedure as that of (17).

3. Model description and experiment design

The LaRC intermediately prognostic higher-order turbulence closure (IP-HOC) scheme assumes a joint double-Gaussian distribution of $\theta^{\text{sub } l^{\wedge}}$, $q^{\text{sub } t^{\wedge}}$ and w (Cheng and Xu 2006). The distribution is inferred from the first-, second-, and third-order moments of these variables and is used to diagnose cloud fraction and grid-mean liquid water mixing ratio, as well as the buoyancy term and fourth-order terms in the equations describing the evolution of the second- and third-order moments. Unlike Golaz et al. (2002a,b), who predict only one third-order moment, IP-HOC predicts three most important third-order quantities, those of $\theta^{\text{sub } l^{\wedge}}$, $q^{\text{sub } t^{\wedge}}$, and w , along with all first- and second-order moments, which gives the scheme its name (i.e., intermediately prognostic). The computational cost of the IP-HOC scheme is about half of the fully prognostic HOC scheme, which predicts all third-order moments.

The IP-HOC scheme is intended primarily for use in situations in which boundary layer clouds are not resolved, with the grid size ranging from a few kilometers (Cheng and Xu 2006, 2008) to the size of a GCM grid box. The scheme has been tested in the University of California, Los Angeles (UCLA)-LaRC cloud-resolving model, where it has greatly improved the simulation of shallow cumulus clouds and produces a gradual transition from shallow to deep convection (Cheng and Xu 2006), and in the System for Atmospheric Modeling (SAM) CRM (Cheng and Xu 2008), where the sensitivity of the boundary layer cloud simulation to horizontal resolution is greatly reduced compared to the standard SAM with a low-order turbulence closure (Khairoutdinov and Randall 2003).

Two Global Energy and Water Cycle Experiment (GEWEX) Cloud System Study (GCSS) boundary layer cloud cases—the Rain in Cumulus over the Ocean (RICO; Rauber et al. 2007; and <http://www.knmi.nl/samenw/rico/>) drizzling shallow cumulus and the Atlantic Stratocumulus Transition Experiment (ASTEX; Bretherton et al. 1999) drizzling stratocumulus - are simulated with three models: the SAM large-eddy simulation (LES), the IP-HOC SCM with the PDF-based microphysics scheme (SCM-CNTL), and the same SCM using the gridmean profiles to calculate the microphysical process rates (SCM-M). The SAM LES, which was developed in Colorado State University by Khairoutdinov and Randall (2003), uses Kessler's (1969) bulk microphysics scheme. Although SAM LES and the SCMs use similar bulk microphysics schemes, the LES has a horizontal grid size of 100 m and basically resolves the variability of cloud and precipitation processes whereas the SCM targets grid sizes ranging from a few kilometers to hundreds of kilometers, which must parameterize the SGS variability of these processes. The microphysical process rates parameterized by the PDF-based microphysics scheme can be

compared with those from the benchmark LES. If the PDF-based microphysics scheme is able to reproduce the results from LES, the scheme can be used in CRMs and climate models with much coarser resolutions. The comparison between SCMCNTL and SCM-M, on the other hand, can demonstrate the importance of considering SGS variability of cloud and precipitation processes in simulating drizzling boundary layer clouds. The sensitivities of results to the autoconversion time scale ($c^{\text{sub } a}$) and the threshold liquid water mixing ratio for autoconversion ($q^{\text{sub crit}}$) are also investigated by increasing and decreasing these two parameters by 10% or 50% compared to SCM-CNTL for the two cases to be described in detail later (Table 2), respectively.

4. Results

a. The RICO composite shallow cumulus case

A detailed description of the configuration of the RICO composite case can be found online (at <http://www.knmi.nl/samenw/rico/>). Briefly, the initial condition and large-scale advective forcing data of this case are based on a 3-week period from 16 December 2004 to 8 January 2005 in which shallow cumulus convection was active. The combined radiosondes and dropsondes show only a weak inversion with continuous high relative humidity (up to 70%) in the inversion layer and above (not shown). The large-scale heat and moisture tendencies due to horizontal advection, large-scale subsidence, and radiative cooling, which are assumed to be time independent, are prescribed; surface fluxes are calculated with a fixed sea surface temperature of 299.8 K and surface pressure of 1015.40 hPa. The observed (spatially averaged) rainfall rate during the 3-week period is about 0.3 mm day^{-1} . The horizontal grid size used in the LES experiment was 100 m in both the x and y directions, with a domain size of 12.8 km \times 12.8 km. A uniform vertical grid size of 40 m was used, with a domain depth of 4 km. The total integration time was 24 h. The vertical grid spacing and the domain depth of the SCM experiments were the same as in the LES experiment.

1) DIAGNOSED AND PREDICTED MICROPHYSICAL PROCESS RATES

A two-step evaluation of the PDF-based microphysics scheme proposed in section 2 is performed. The diagnostic test utilizes the hourly-mean first-, second-, and third-order moments diagnosed from the LES experiment and related information from the assumed PDF to compute the autoconversion, collection, and evaporation rates using the analytical expressions derived in section 2, which are then compared to those diagnosed directly from the LES experiment described in section 3. The LES results will be treated as "benchmarks" although the microphysics scheme used in the LES is rather simple. The prognostic test results are obtained from the SCM-CNTL experiment (see section 3). Both sets of results shown in Fig. 1 are averaged over the last 6 h because cumulus clouds, as shown later, reach a more quasi-steady state compared to the earlier periods of the integration.

First, the magnitudes and the overall vertical shapes of all three diagnosed microphysical process rates from the PDF-based scheme compare well with those diagnosed directly from LES, except for some differences noted below. The collection rates from the LES and the diagnosis are about 5 times higher than the autoconversion rates in the cloud layer and the evaporation rates in the cloud layer are generally higher than the autoconversion rates and increase rapidly toward the surface. Second, both the collection and autoconversion rates are underestimated in the upper cloud layer (i.e., 1800-3200 m). The magnitudes of the overestimates of these rates in the lower part of the cloud layer (i.e., 900-1600 m) are smaller than those of the underestimates in the upper cloud layer. The main reason for this result is that the double-Gaussian-based PDF approach cannot represent the distribution near the cloud top with large skewness (sometimes >100) simulated by the LES. Thus, the Gaussian-mean liquid water mixing ratio obtained using smaller skewness is underestimated, which leads to an underestimate in the autoconversion fractional area, rainwater mixing ratio, and microphysical process rates for each Gaussian. Larson et al. (2005) noticed the same discrepancy using a similar approach (see their Figs. 4 and 5). Finally, the evaporation rates are well parameterized, including the reproduction of the minimum near the cloud base. This result is probably related to the fact that the parameterized evaporation rate

depends highly on relative humidity and saturation specific humidity. Both come from the LES in the diagnosis. The effects of the correlation between $q^{\text{sub } x^{\wedge}}$ and the rainwater mixing ratio (...) on the collection and evaporation rates can be seen by comparing the diagnosed rates that include or exclude the correlation terms in (10) and (14) denoted by SCHM and SCHM-NOCOR in Figs. 1a,b, respectively. Based on the definition of $q^{\text{sub } x^{\wedge}}$ given in (4), a positive $q^{\text{sub } x^{\wedge}}$ is identical to $q^{\text{sub } l^{\wedge}}$ (condensation) whereas a negative $q^{\text{sub } x^{\wedge}}$ corresponds to $q^{\text{sub } v^{\wedge}} - q^{\text{sub } s^{\wedge}}$ (saturation deficit). As seen from Fig. 1b, the positive correlation between $q^{\text{sub } x^{\wedge}}$ and q_i of each Gaussian enhances the collection rate in the middle of the cloud layer, which improves the agreement with the LES. On the other hand, the positive correlation between the saturation deficit and $q^{\text{sub } r^{\wedge}}$ of the Gaussian enhances the evaporation rate in the cloud layer because a more unsaturated environment evaporates more rainwater. This correlation reduces the evaporation rate significantly between 1000 and 2500 m and slightly improves the agreement with the LES but does not change the diagnosed values in the subcloud layer.

The interactive test (from the SCM-CNTL experiment) overall shows similar results to the diagnosis (Figs. 1a-c). However, there are slightly larger overestimates in the autoconversion and collection rates in the lower part of the cloud layer than in the diagnostic test. This result is related to the excessive liquid water and the lower cloud-base height (Figs. 2c,d). The underestimate in the autoconversion and collection rates in the upper cloud layer is only slightly larger than in the diagnostic test. The interactive test has the greatest impact on the magnitude of the evaporation rate because of slight differences in the thermodynamic soundings in the cloud and subcloud layer from the LES (Figs. 2a,b).

The time series of the relative error of the microphysical process rates between SCM-CNTL and LES, defined by $|(I^{\text{sub } \text{SCM}^{\wedge}} - I^{\text{sub } \text{LES}^{\wedge}})/I^{\text{sub } \text{LES}^{\wedge}}|$, where $I = \int^{\wedge}_{\text{sup } Z^{\wedge}} \text{t}^{\wedge} \text{sub } 0^{\wedge} r \text{ dz}$ is the vertically integrated rates and r is the microphysical process rate, are shown in Fig. 1d. The relative errors between the SCM-CNTL and LES are generally less than 10%. The relative error for the evaporation rate has the smallest magnitude among the three rates because of its dependence on the mean thermodynamic profiles, which have relatively smaller differences between SCM-CNTL and LES than the liquid water and rainwater mixing ratios do.

The relative errors in these process rates arise mainly from deficiencies in the double-Gaussian representation of SGS variability in the IP-HOC discussed in this study. The differences between the microphysical process rates for formulas used in the LES and SCM-CNTL (e.g., the Kessler versus Sundqvist autoconversion rates) do not impact the errors substantially (not shown).

2) MEAN PROFILES AND CLOUD EVOLUTION

Figure 2 shows the mean profiles of potential temperature, total water mixing ratio, liquid water mixing ratio, and cloud fraction averaged for the last 6 h of the LES, SCM-CNTL, and SCM-M integrations. In general, the profiles obtained from SCM-CNTL agree better with those of the LES than those obtained from the experiment without considering the SGS variability (SCM-M). SCM-M overestimates the inversion height, cloud-top height, and cloud fraction near the cloud top (1800-2700 m), compared to the LES and SCM-CNTL. The good agreement with LES in liquid water mixing ratio in the upper cloud layer arises from the overestimated cloud fraction in SCM-M (Note that the underestimate of liquid water mixing ratio in SCM-CNTL arises from the underestimate of cloud fraction in the same region of the cloud layer). Understanding the cause for the overestimates in SCM-M is beyond the scope of this study, but they could be due to the strong cloud-top entrainment and the lack of precipitation processes.

There are, however, some problems common to the two SCM experiments related to the turbulence parameterization. For example, both SCMs underestimate the total water mixing ratio in the subcloud layer (Fig. 2b) and overestimate the liquid water mixing ratio near cloud base (Fig. 2c), which may be caused by the efficient transport of moisture in subcloud layer (not shown). The overestimate of liquid water mixing ratio near cloud base influences the microphysical processes such as autoconversion and collection, as shown in Figs. 1a,c. It is worth mentioning that the small liquid water mixing ratio and cloud amount (Figs. 2c,d) for this case

inhibit autoconversion and the associated microphysical processes using the approach proposed by Bechtold et al. (1993). This is also the case in the SCM-M experiment.

To further understand the autoconversion processes, profiles of the fractional area of autoconversion (f_{cr}^{\wedge}) and the standard deviation of q_{x}^{\wedge} (i.e., σ_{s}^{\wedge}) averaged over last 6 h are shown in Fig. 3. In the SCM, f_{cr}^{\wedge} is diagnosed using Eq. (7) whereas it is directly diagnosed from the LES grid points at a given height where autoconversion occurs. It is interesting to note that f_{cr}^{\wedge} is about an order of magnitude smaller than the cloud fraction (Fig. 2c). The autoconversion processes occur most often in the middle of the cloud layer in the LES, but at an altitude close to the cloud base in the SCM (Figs. 3a and 1c). The more frequent occurrence of autoconversion near the cloud base in SCM is related to both the 50% overestimate of liquid water mixing ratio in the SCM (Fig. 2c) and the wider distribution of saturation implied by large values of σ_{s}^{\wedge} between 800 and 1600 m, compared to the LES (Fig. 3b). The magnitudes of σ_{s}^{\wedge} , from LES and SCM-CNTL agree well with each other elsewhere.

The rainwater mixing ratio and its standard deviation are important for understanding the rainwater collection and evaporation. Their vertical profiles averaged over last 6 h are shown in Fig. 4. The agreement between LES and SCM-CNTL is fair at most heights, but there are large underestimates in the upper portion of the cloud layer. This is due partly to the large skewness that cannot be captured by the assumed PDF. The sub-cloud layer evaporation tends to decrease the rainwater mixing ratio toward the surface for SCM-CNTL but not for LES (Fig. 4a). The standard deviation of rainwater mixing ratio, which is smaller than the grid-mean rainwater mixing ratio, agrees between SCM-CNTL and LES in the lower region of the cloud layer and the subcloud layer. The effects of rainwater perturbation on collection and evaporation as expressed by (10) and (14) are to increase collection and evaporation when correlated with the liquid water mixing ratio and environmental saturation deficit, respectively.

The time series of the cloud fraction (Fig. 5) provides us with some information on the evolution of the shallow cumulus clouds between the LES and SCM experiments. The largest cloud fraction is about 6% and is located near 600 m. The cloud top continues to rise toward the end of the integration for LES and SCM-CNTL (except for a dip at 17 h for SCM), but more quickly for the SCM-M. The cloud fraction near the cloud top from the SCM-M run is larger than that from the SCM-CNTL and LES runs for the last 12 h of the simulations. According to Fig. 2c, the grid-mean liquid water mixing ratio is much less than q_{crit}^{\wedge} so there is no autoconversion (and associated microphysical processes) for SCM-M. The lack of the processes that deplete the liquid water and produce precipitation may cause the larger cloud amount near cloud top for SCM-M.

3) SENSITIVITY TESTS

A drawback of the Kessler and Sundqvist-type auto-conversion formulas is that they are not linked to the microphysical parameters such as the size and number concentration of cloud droplets but rather depend on two empirical parameters: the autoconversion time scale (c_{a}^{\wedge}) and the minimum liquid water mixing ratio for autoconversion (q_{crit}^{\wedge}). However, they are very simple and the analytical expressions can be easily obtained using the PDF approach. They are ideal formulas for the first-step extension of the IP-HOC to include microphysical processes.

To understand the sensitivities of the autoconversion rate to c_{a}^{\wedge} and q_{crit}^{\wedge} , four more experiments were made based on SCM-CNTL (Table 2). Results from the tests (Fig. 6) show that dependence of autoconversion rate on these parameters is basically nonlinear. The corresponding changes in collection and evaporation rates are also large (not shown).

b. Long-term experiment for the RICO shallow cumulus case

The long-term run for the RICO shallow cumulus case covered the period from 16 December to 8 January 2005 when shallow cumulus clouds were active and was designed specifically for an SCM intercomparison study. The initial condition is based on the soundings of 16 December. A prescribed sea surface temperature decreases linearly from 300.2 K on 16 December to 299.6 K on 8 January 2005. The time-varying large-scale

forcings, such as horizontal and vertical advection of wind, temperatures and moisture, are also prescribed. The temperature tendency due to radiation processes is not given, so an interactive radiation scheme (Xu and Randall 1995) was implemented in the SCM to take the effects of radiation into account. The vertical grid spacing and domain depth are the same as in the composite case discussed in section 4a.

The SCM with the PDF-based microphysics scheme is stable for the entire 3-week period, producing heavy drizzle rates of 2-6 mm day⁻¹ to light drizzle rates less than 0.1 mm day⁻¹ (Fig. 7a), with a period average of 0.28 mm day⁻¹ (close to the observation of 0.3 mm day⁻¹). The observed precipitation rate (dotted line) is derived from an S-band polarimetric radar, which was located on the island of Barbuda and was operational continuously for the full RICO campaign. The microphysical process rates in the long-term experiment are overall larger than those in the composite experiment. The maximum magnitudes of autoconversion, collection, and evaporation rates (Fig. 8) from the long-term run are about 2 times larger than those from the composite run (Fig. 1). The largest autoconversion rate near cloud top (at 3700 m) is associated with larger cloud fraction (more than 40%; not shown), but autoconversion occurs more frequently near 2000 m for most of the shallow cumulus clouds. The collection also occurs frequently and has its largest magnitude near 2000 m (Fig. 8b), which is also the height of the maximum autoconversion and collection for the composite experiment. The evaporation, on the other hand, occurs at all levels below 3700 m and usually has its largest value at the surface.

To further understand the long-term effects of precipitation processes, the differences in the TKE, surface sensible and latent heat fluxes between the SCM-CNTL and SCM-M long-term experiments are shown in Figs. 7b-d. The column-integrated TKE usually decreases during drizzling subperiods (e.g., days 3 and 11). The evaporative cooling and moistening effects of drizzling increase the surface sensible heat flux but decrease the surface latent heat flux during precipitating subperiods.

c. A stratocumulus case

A stratocumulus case with light drizzle was configured based on the ASTEX observations (de Roode and Duynkerke 1997), which represent a typical stratocumulus topped boundary layer. The prescription of de Roode and Duynkerke (1997) is followed. The observed cloud deck had a thickness of 500 m, extending from 300 to 800 m. The temperature jump was 5.5 K at the inversion. The simulations are initiated with an adiabatic liquid water mixing ratio profile, with a peak value of -0.7 g kg^{-1} . Surface sensible and latent heat fluxes are prescribed. A simple interactive radiation scheme is included (Stevens et al. 2001). Each simulation lasts for 3 h, beginning at 0400 UTC 13 June 1992. For the LES, the horizontal grid spacing was 50 m in both the x and y directions, with a domain size of 3.2 km \times 3.2 km. A uniform vertical grid spacing of 25 m was used, with a domain depth of 1.5 km. The vertical domain depth and integration time for the SCM are identical to the LES. The overall evolution (Fig. 9) of cloud fraction from all three (LES, SCM-CNTL, and SCM-M) simulations is very similar; they do produce realistic overcast cloud deck between 300 and 800 m and the cloud top tends to increase gradually toward the end of integration. Minor differences can be noticed at the bottom and the top of cloud layer.

The autoconversion, collection, and evaporation rates (Fig. 10) from the LES and SCM-CNTL runs are about one order of magnitude smaller than those from the RICO cases. Unlike the cumulus case, the peak magnitudes of all three rates are comparable. The collection and evaporation rates from the SCM still compare well with those from LES. There is no evaporation within the cloud deck, as expected. The autoconversion is overestimated in magnitude and is nonzero throughout the cloud layer in the SCM, compared to the LES. The inhomogeneity of the stratocumulus clouds seems to play an important role in the microphysical processes because the deck of 100% cloud fraction extends from 300 to 800 m (Fig. 9), but autoconversion only occurs near the center of the cloud deck. The grid-mean liquid water mixing ratio is less than $q^{\text{sub crit}}$ (Fig. 11c), so there is no autoconversion for the approach proposed by Bechtold et al. (1993) and SCM-M, and the associated microphysical processes do not occur in SCM-M.

Because of the small magnitudes of autoconversion, collection, and evaporation, the differences between SCM-CNTL and SCM-M on potential temperature θ , total water mixing ratio q^* and cloud fraction almost cannot be distinguished in Fig. 11. The dashed line for SCM-CNTL and the dotted line for SCM-M almost overlap to a dashed-dotted line. The liquid water mixing ratio from SCM-CNTL, however, is less than that from SCM-M because of the conversion of liquid water to rainwater from the microphysical processes. There is also a common problem resulting from the turbulence parameterization for SCM experiments. The gradient of θ and q^* is not maintained because the SGS fluxes are underestimated for the two simulations. This result agrees with Zhu et al. (2005), who showed that some SCMs tend to smooth out the sharp jumps of θ and q^* at the cloud top and have large gradients in θ and q^* within the mixed layer. They suspected that the SCM inversion structure depends on details of its turbulent parameterization—in particular, the cloud-top entrainment.

Because of the smoothing of the large gradients of the mean thermodynamic profiles near cloud top by SCM-CNTL, the standard deviation of q^* (σ^*) from SCM-CNTL is underestimated at the upper half of the cloud layer but overestimated above the LES cloud top and the lower half of the cloud layer (Fig. 12b). The underestimated σ^* can weaken autoconversion due to more homogeneous spatial distribution but increase the autoconversion area (Fig. 12a), which enhances autoconversion (Fig. 12). These two effects may be cancelled out at the upper half of the LES cloud layer. The overestimated σ^* at the lower half of the cloud layer clearly increases autoconversion [last term in (6)] while the area of autoconversion is also increased because of the increase of the grid-mean liquid water.

As in RICO, the sensitivities of the autoconversion rate to the autoconversion time scale are nonlinear (Fig. 13); a 10% change of τ_{cril} causes a 50% variation of autoconversion rate. It is possible that the SGS distribution of liquid water mixing ratio changes as the value of q_{crit} changes from its default value. This again suggests the weakness of the Kessler and Sundqvist-type parameterizations that are highly dependent upon τ_{cril} and are difficult to further generalize. More sophisticated schemes, such as double-moment microphysics, are needed for the IP-HOC SCM and benchmark LES, which will be left as future work.

5. Discussion and conclusions

In this study, a warm-rain microphysics parameterization that is based on the SGS distribution of vertical velocity, liquid water potential temperature, total water mixing ratio, and perturbation of rainwater mixing ratio has been developed to simulate drizzling boundary layer clouds. The assumed PDF is a joint double Gaussian and its parameters are determined from the moments of a higher-order turbulence closure scheme at each time step (Cheng and Xu 2006). The PDF is used to derive analytical expressions for autoconversion, collection, and evaporation rates in the warm-rain microphysics parameterization. The analytical expressions show that correlation between rainwater and liquid water mixing ratios of the Gaussian enhances the collection rate whereas that between saturation deficit and rainwater mixing ratios enhances the evaporation rate. The autoconversion, collection, and evaporation rates diagnosed from LES input moments and predicted from the SCM compare well with those obtained from the benchmark LES for drizzling cumulus and stratocumulus cases.

The SAM LES, SCM-CNTL, and SCM-M have simulated cases of drizzling shallow cumulus and stratocumulus with the bulk microphysics schemes. The LES has a horizontal grid size of 100 m or less and basically resolves the variability of cloud and precipitation processes, whereas the SCM targets grid sizes ranging from a few kilometers to hundreds of kilometers, which must parameterize the SGS variability of these processes. Two SCM experiments were performed for each case, one with the IP-HOC SCM using the PDF-based microphysics scheme (SCM-CNTL), and the other with the same SCM using the grid-mean profiles to calculate the microphysical process rates (SCM-M). A main goal of the testing of the PDF-based microphysics scheme is to reproduce the results from LES so that the new scheme can be used in CRMs and climate models with much coarser resolutions. Although the results from SCM-CNTL were influenced by the underlying turbulence

parameterization, SCM-CNTL can reproduce the autoconversion, collection, and evaporation from LES well for the shallow cumulus and stratocumulus cases. The comparison between SCM-CNTL and SCM-M, on the other hand, showed the improvements in mean profiles of potential temperature, total water mixing ratio, liquid water mixing ratio, and cloud amount in the experiment considering the SGS variability. A 3-week integration using the PDF-based microphysics scheme indicates that the new scheme is stable for long-term simulations.

Sensitivity tests to the autoconversion time scale and the minimum liquid water mixing ratio for autoconversion show that the autoconversion may change nonlinearly with a linear variation of the two parameters. This suggests a limitation of the Kessler and Sundqvist-type autoconversion formulas, which are difficult to further generalize. However, given the extensive usage and simplification of the formulas, it is still a good idea to use them for a first-step extension of the IP-HOC to include a PDF-based microphysics scheme.

The present work opens doors to some exciting future research opportunities. The majority of microphysics parameterizations currently used in CRMs and climate models neglect all SGS variations and calculate the effect of all cloud and precipitation processes as if the gridbox vertical velocity, temperature, moisture, and rainwater mixing ratio should be uniform [with some exceptions such as Zhang et al. (2002)]. This may cause systematic biases as shown by Larson et al. (2001a) and Woods et al. (2002). Zhang et al. (2002) only considered the SGS variability of liquid water mixing ratio. The method used in this study can be generalized to include microphysical processes for ice, snow, graupel, etc., because the SGS PDF contains all the necessary information to remove such biases.

Another important microphysical process is the interaction of turbulence on cloud condensation nuclei (CCN) and ice-forming nuclei (IFN). The CCN and IFN activation depends highly on local supersaturation and inhomogeneity, which, in turn, depend on local SGS distribution and turbulence. The local supersaturation can differ dramatically even on a scale of a few kilometers, but CRMs and climate models typically use grid-mean values. Thus, significant errors can occur if the SGS variability is ignored. The assumed PDF provides valuable information for improving the activation of CCN and IFN. This requires a PDF-based microphysics scheme that includes the number concentrations of water species in addition to mixing ratios of cloud, ice, rain, snow, and graupel.

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