Multimoment Ice Bulk Microphysics Scheme with Consideration for Particle Shape and Apparent Density. Part I: Methodology and Idealized Simulation

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ABSTRACT

To improve the parameterization of ice-phase microphysics in regional meteorological models, this study developed a triple-moment bulk scheme, which also tracks the variations in the shape and density of several hydrometeors. Solid-phase hydrometeors are classified into pristine ice, snow aggregates, rimed ice, and hailstones based on their physical mechanisms. The new scheme has been incorporated into the Weather Research and Forecasting Model and tested with an idealized two-dimensional simulation of a squall-line system. The simulation successfully revealed the smooth transition from the convective core to the stratiform anvil as well as the alternating pattern in the hydrometeor vertical distributions, as was similarly demonstrated in other similar studies. A few sensitivity tests were performed to reveal the importance of including shape and density variations, which strongly affect the mean particle size by up to 50% and fall speed by as much as 100% for individual hydrometeor categories. Furthermore, the inclusion of a third moment could enhance the diffusional growth rate of small crystals and reduce the ventilation effect of large particles compared with the conventional double-moment approach. These factors have a significant influence on cloud structure and precipitation amounts.

1. Introduction

Enabled by increasing computer power, there is an increasing need to apply explicit cloud microphysics schemes with more detailed physics and mathematics to better represent cloud and precipitation processes in regional meteorological models (Tao and Moncrieff 2009). In particular, the parameterization of ice microphysics is important in simulations of microphysical–dynamical interaction (e.g., Leary and Houze 1979; McFarquhar et al. 2006), cyclone evolution (e.g., Tao et al. 2011; Jin et al. 2014; Dearden et al. 2016), meso-scale convective systems (e.g., McCumber et al. 1991; Van Weverberg et al. 2013), cloud radiative properties (e.g., Gu and Liou 2000; Yang and Fu 2009), and

quantitative precipitation forecasts (e.g., Gilmore et al. 2004; Thompson et al. 2008). However, the wide variety of ice crystals in terms of size and morphology makes it rather difficult to describe them realistically in cloud modeling. Although there still exist many uncertainties in ice-phase nucleation/growth, a large part of the difficulties in cloud microphysics modeling resides in the representation of hydrometeors' size distributions and physical properties (e.g., shape and density), which are the focuses of this study.

Both bulk and bin methods have been used to describe the size distributions for representing cloud microphysical processes in numerical models. The bin method explicitly predicts the evolution of particle size distributions, whereas the bulk approach usually specifies a functional form for the size distribution for each hydrometeor category. However, the bin method has yet to demonstrate its superiority over the bulk method in all types of cloud simulations (cf. Xue et al. 2017; Yin et al. 2017). With the advantage of computational efficiency, the bulk method continues to be a

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more practical approach than the bin method being applied to regional models. The bulk methods originated from the one-moment (1M) scheme of Kessler (1969), which predicts the rate change of cloud drop and raindrop mass mixing ratios. Later schemes have included ice-phase hydrometeor categories (e.g., Cotton et al. 1982; Lin et al. 1983; Rutledge and Hobbs 1984; Dudhia 1989; Tao and Simpson 1993). More detailed two-moment (2M) schemes have emerged for predicting both the mass and number mixing ratios (Meyers et al. 1997; Reisner et al. 1998; Thompson et al. 2004; Morrison and Pinto 2005; Seifert and Beheng 2006). Subsequently, Milbrandt and Yau (2005b, hereinafter MY05b) and Loftus et al. (2014) have proposed relatively sophisticated three-moment (3M) schemes, using radar reflectivity factor (only proportional to the sixth moment of the size distribution with constant density spherical particles) as the additional moment. Morrison et al. (2009) pointed out the advantage of 2M over 1M schemes being used to reduce excessive rain evaporation and to produce better precipitation structures in squall lines. Milbrandt and Yau (2005a, hereinafter MY05a) have demonstrated that the inclusion of a third moment may significantly affect the instantaneous growth rates and fall velocities. In a parcel-type calculation, Chen and Tsai (2016, hereinafter CT16) demonstrated that the 3M method can simulate well the evolution of ice crystal size distribution during vapor deposition, compared against the bin model calculations, whereas the 2M representation may cause 37% underestimation in overall mass growth for 1000 s under water saturation.

In addition to the problem in the moment-type representation of ice-particle size spectra, the external (e.g., aspect ratio) and internal (e.g., porosity) morphologies of ice crystals are another complicated issue and are often crudely represented in microphysical schemes. Most of the earlier microphysics schemes assumed that ice crystals are spherical with a constant apparent density (mass divided by circumscribed volume, which includes hollows, pores, and notches). Efforts have also been devoted to avoid using constant density for snow by applying a mass–dimension relation, which implies an inverse relationship between size and apparent density (Thompson et al. 2008; Milbrandt et al. 2008); however, in reality, shape and apparent density vary significantly and have many consequences in nearly all microphysical processes. For example, using the spherical assumption may underestimate the vapor deposition rate (Chen and Tsai 2016) or overestimate the fall speed (Böhm 1992; Khvorostyanov and Curry 2002; Mitchell and Heymsfield 2005) by several folds. Sulia et al. (2014) showed the impact of ice adaptive habit on the microphysical evolution during Arctic mixed-phase cloud glaciation. Shape

also strongly affects ice particle collision efficiency (Böhm 1999; Wang and Ji 2000), optical properties (Yang and Fu 2009), and radar scattering cross section (Molthan and Petersen 2011; Ryzhkov et al. 2011; Sulia and Kumjian 2017).

Some studies have attempted to include shape effects in microphysical calculations, such as utilizing simple fixed mass–dimension (m - D) and terminal velocity–dimension (v - D) relationships pertaining to a specific shape of ice particles (e.g., Ji and Wang 1999; Hong et al. 2004; Avramov and Harrington 2010), but the past history of shape was ignored in these schemes. Straka and Mansell (2005) determined the habit of new ice crystal being either columns or plates from ambient temperature, but their height–length and mass–dimension relationships were held constant. Harrington et al. (2013) followed a theoretical parameterization of Chen and Lamb (1994a, hereinafter CL94a) to develop an adaptive growth habit 2M method by tracking two mean axis lengths of ice crystals. Their parameterization allows the growth habit of ice crystals to evolve in a realistic manner by considering feedback between changes in the ice shape and diffusional mass growth. A similar ice crystal shape parameterization was proposed later by CT16, but it tracks the ice crystal aspect ratio instead of individual axis lengths, and the mixture of habits is considered implicitly with the volume-weighted bulk aspect ratio. CT16's parcel-type calculations revealed that a realistic transition of size-dependent adaptive habit against distinct environmental conditions and the derived results using a 3M parameterization was very close to binned calculations. More recently, Jensen et al. (2017) modified the scheme of Harrington et al. (2013) to track two volume-dimensioned mixing ratios and also extended the bulk framework to a new scheme called the Ice-Spheroids Habit Model with Aspect-Ratio Evolution (ISHMAEL) by considering planar and columnar ice as two separate ice categories (such that different habits may coexist) and by treating aggregates as a separate ice species.

In addition to the deposition growth, many modeling studies have continuously made improvements in the physical parameterization of ice riming processes. Morrison and Grabowski (2008) proposed an approach to predict the rimed mass fraction by tracking ice mixing ratios separately from deposition and riming growth. Lin and Colle (2011) used a diagnosed riming intensity to account for the effects of partially rimed crystals by the m - D , projected area–dimension (A - D), and v - D relationships. Based on the work of Connolly et al. (2006), Mansell et al. (2010), and Milbrandt and Morrison (2013) further added a prognostic volume variable to predict the graupel bulk density. Furthermore, Morrison and Milbrandt (2015) developed a new predicted particle properties (P3) bulk scheme to

predict the rime mass fraction and the bulk density for a single ice category (but options for more categories are available). Note that the influence of density on ice fall speed was included in the P3 scheme through a theoretical parameterization of Mitchell and Heymsfield (2005, hereinafter MH05). Jensen and Harrington (2015, 2017) also predict the change in ice particle shape during riming. However, these previous schemes did not focus on a detailed treatment of aggregation. A tentative method to diagnose snow density was adopted separately by Thompson et al. (2008) and Lang et al. (2014) according to a size-dependent and mass-mapping relation. Subsequently, Geresdi et al. (2014) considered size-dependent relations over different diameter intervals for the shape and density of dry snowflakes in their bin microphysical scheme, as well as a linear interpolation between partially melted snow particles and raindrops. Although such treatment is empirical in nature, it cannot be applied easily to bulk schemes.

In earlier bulk cloud schemes, ice-phase hydrometeors were typically divided into small nonprecipitating cloud ice and large precipitating ice such as snow or graupel. The conversions of cloud drops to raindrops or cloud ice to precipitating ice particles were conditional upon arbitrary size or mass thresholds. For example, a certain amount of mass acquired from deposition, riming, and aggregation growths of ice crystals was transferred as snow or graupel embryo through a threshold-size (or mass) calculation (e.g., Lin et al. 1983; Murakami 1990; Reisner et al. 1998); thereby, the snow category in effect contained a mixture of large pristine ice, rimed crystals, and aggregates that are quite different in their morphology. Similarly, a given embryo mass was also applied to graupel initiation from cloud ice or snow particles under heavy riming, and the amount of conversion is typically determined by ad hoc or tunable parameters. In such bulk schemes, the definitions of cloud ice, snow, and graupel categories are often vague without observational justification (Schmitt and Heymsfield 2014), and conversions among them are strongly regulated by arbitrary thresholds, which could result in unnatural behaviors among these solid hydrometeors (Morrison and Grabowski 2008; Eidhammer et al. 2014).

The implementation of a threshold limit implies a discontinuity in the size distribution (cf. Fig. 1), a factor commonly ignored when deriving the bulk conversion rates. Although an incomplete integral derivation can be used to account for the size discontinuity (e.g., Harrington et al. 1995), the assumption of a threshold size is still not physically based. Morrison and Milbrandt (2015) discarded the traditional categorization of ice-phase hydrometeors and applied a single free ice category in their P3 scheme to avoid the problems of conversion between solid hydrometeors; however, ice particle vapor growth is constrained

FIG. 1. Schematics of threshold problems in the Marshall–Palmer-type size distribution. (a) The distribution of cloud ice after certain growth, and part of the distribution exceeded the size threshold r^* . With the “autoconversion” process, the distribution is divided into (b) the cloud ice portion and (c) the snow portion (solid lines). To maintain a continuous inverse exponential distribution, the two new sections need to be redistributed as represented by dashed lines, which inevitably will violate the threshold definition.

by mass–dimension relationships that are chosen empirically. Later, the P3 scheme was extended to offer a user-specified number of ice-phase categories by Milbrandt and Morrison (2016). However, whether such a simplified scheme can effectively account for the vast complexity of ice-phase hydrometeors’ shape remains to be proven.

Motivated by deficiencies in current bulk schemes, as mentioned above, and the paradigms set by the later development in microphysical schemes (e.g., P3 and ISHMAEL), this study intends to implement the ice crystal 3M parameterization developed by CT16 into a bulk cloud model with consideration of the adaptive growth habit and apparent density, together with a triple-moment closure approach that allows for size distribution to evolve with a higher degree of freedom. The influence of crystal shape and density on all ice-related collection processes such as riming and aggregation are considered. Furthermore, hydrometeor types are redefined based on their formation mechanisms to reduce ambiguity in the growth process and uncertainty in conversion thresholds. The formulation of microphysical processes relevant to the above considerations was also improved accordingly. In the following, we describe the concept behind this new bulk parameterization, the triple-moment closure scheme, the treatment of ice-phase hydrometeors’ shape and density, and its overall performance when implemented into the Weather Research and Forecasting (WRF) Model to simulate a two-dimensional idealized squall-line system.

2. Scheme description

a. Hydrometeor categories

Following the conventional bulk method, our scheme categorizes liquid-phase hydrometeors into cloud drops (CDs) and raindrops (RDs); however, for ice-phase

hydrometeors, a different categorization is applied. The traditional “cloud ice” category is redefined as “pristine ice” (PI) particles, which grow solely by vapor deposition and without an upper size limit. In this way, there is no need to use the artificial “auto-conversion” process to convert large cloud ice into snow, as is done in traditional schemes. It also avoids the mathematical problem of handling the discontinuity in size spectrum due to cutoff size, as illustrated in Fig. 1.

In traditional bulk schemes, the elimination of cloud ice “autoconversion” will deprive the source of snow. This problem is avoided by redefining snow as “snow aggregate” (SA), which originates only from the self-aggregation of PI and only grows through vapor deposition, PI collection, and SA self-aggregation. The riming growth on PI and SA results in the next category called the “rimed ice” (RI), which is similar to the traditional “graupel” category. This RI initiation is performed with a “cash advance” approach, where the mass acquired during riming is converted immediately to RI along with an equal amount of the collector mass, such that the RI is always “heavily” rimed. For example, if PI collects cloud drop mass that is 10% of its own weight, then 10% of the PI is converted to RI along with the collected cloud drops. Other initiation and growth processes of RI follow the conventional method. RI interacts hydrodynamically (e.g., collisional processes) only with liquid-phase hydrometeors. The hailstones (HS) category is initiated from graupel when the growth condition reaches the Shumann–Ludlam limit (SLL; Ziegler 1985; Young 1993) during heavy riming. This SLL criterion indicates that the spectrum-discontinuity problem shown in Fig. 1 still exists in the conversion between RI and HS categories. Nevertheless, the discontinuity problem is less significant when the three-moment gamma distribution is applied, as it allows the adjustment of the spectral shape at both ends of the size spectrum.

The modifications in the hydrometeor category definition applied here allow a clearer association of physical processes with the categories, which is important to further improvements in bulk microphysics.

b. Size distribution and its moments

The size spectrum (number density function) of a given ice-phase hydrometeor category is represented here using a three-parameter gamma distribution function in the following form:

$$n(D) = N_0 D^\alpha e^{-\lambda D}, \quad (1)$$

where D is the diameter of an equivalent volume sphere, and N_0 , α , and λ are called the intercept, spectral dispersion, and slope parameters, respectively.

The distribution parameters (N_0 , α , and λ) are not extensive properties and thus cannot be used directly as prognostic variables. Suitable prognostic variables are the “moments” of the distribution function, which are defined as follows:

$$M_j = \int D^j n(D) dD. \quad (2)$$

Note that the integration limits are always 0 to ∞ but are omitted in the equations throughout the text. This study applied three moments to describe the size distribution, including the zeroth ($j = 0$), second ($j = 2$), and third ($j = 3$) moments, respectively representing the mixing ratio of number N ($=M_0$), cross-section area A [$=(\pi/4)M_2$], and volume V [$=(\pi/6)M_3$]. Note that some schemes selected M_6 (e.g., MY05b; Loftus et al. 2014), but here we selected M_2 as the third moment because the second moment is proportional to the cross-section area, which has direct relevance to the collision processes, fall speed calculation, and crystal shape determination. Also, the second moment is an important parameter in calculating cloud radiative fluxes, which may feedback to cloud dynamics; in contrast, the sixth moment is useful for comparing with radar observations but has no direct bearing on cloud microphysical processes except through its influence on the size distribution.

The prognostic variables (including the moments) and diagnostic properties of the six hydrometeor categories are summarized in Table 1. Note that the 2M warm cloud scheme used here lacks M_2 , which may be needed in calculating certain mixed-phase processes. Therefore, we utilized the diagnostic formula for effective radii ($r_e \equiv M_3/2M_2$) from Chen and Liu (2004) to obtain M_2 for cloud drops and raindrops when required. By applying the gamma distribution in Eq. (1) for $n(D)$, the analytical solution to Eq. (2) can be derived as follows:

$$M_j = \frac{N_0 \Gamma(j + \alpha + 1)}{\lambda^{j+\alpha+1}}, \quad (3)$$

where Γ is the Euler gamma function. A closure condition for the spectral parameters in Eq. (1) can be made by applying Eq. (3) to derive the following (cf. CT16):

$$\alpha = \frac{6 - 3q + \sqrt{q(q+8)}}{2(q-1)}, \quad (4a)$$

$$\lambda = \left[\frac{M_0 \Gamma(\alpha + 4)}{M_3 \Gamma(\alpha + 1)} \right]^{1/3} \quad \text{or} \quad = \frac{(\alpha + 3)M_2}{M_3}, \quad (4b)$$

$$N_0 = \frac{M_0 \lambda^{\alpha+1}}{\Gamma(\alpha + 1)}, \quad (4c)$$

TABLE 1. Classification of hydrometeor types and associated particle properties, including the prognostic moments, the treatments of particle shape and apparent density, and the range of spectral dispersion α .

Hydrometeor type		Moments	Shape	Density (kg m^{-3})	Range of α
CD	Cloud	Q, N	Spherical	1000	0–2996
RD	Rain	Q, N			0–2996
PI	Pristine ice	Q, N, A, V, F	Aspherical	50–910	3–2996
SA	Aggregates	Q, N, A, V, F			0–2996
RI	Rimed ice (graupel)	Q, N, A, V	Spherical	50–900	0–2996
HS	Hail	Q, N, A		900	0–2996

where $q \equiv M_0 M_3^2 / M_2^3$.

In addition to the three moments (i.e., M_0 , M_2 , and M_3) that are used to determine size distribution, our scheme also tracks two additional hydrometeor properties, the first of which is water mass mixing ratio:

$$Q = \bar{\rho} V = \bar{\rho} \frac{\pi}{6} M_3, \quad (5)$$

where $\bar{\rho}$ is the mean density. The rate change of Q is associated with the rate change of volume (or M_3) as the following:

$$\frac{dQ}{dt} = \rho_{\text{ap}} \frac{dV}{dt}, \quad (6)$$

where the proportionality constant ρ_{ap} is the apparent density of the added volume, which is a function of temperature and vapor density excess (cf. CL94a). The consideration of both Q and V for PI, SA, and RI allows these hydrometeors to have variable apparent density. The second property is the “bulk shape,” defined as a volume-weighted (or more precisely, third-moment-weighted) aspect ratio:

$$F \equiv \int \phi D^3 n(D) dD, \quad (7)$$

where $\phi \equiv c/a$. For PI, c is the semidimension perpendicular to the basal faces, and a is the semidimension toward a corner of the hexagon. For SA, c is the short axis and a is the long axis. In this study, only PI and SA categories are considered to have shape variations, and for both the spheroidal shape representation following CL94a was applied. For PI, prolate spheroid ($c > a$) represents columnar pristine ice, whereas oblate spheroid ($c < a$) represents planar pristine ice. For SA, the shape is always oblate spheroid. The variations in shape and density are considered in the calculation of fall speed and collision efficiencies (see sections C and D in the online supplemental material). Note that the proposed scheme also tracks dissolved aerosol mass in cloud drops and raindrops to account for aerosol recycling but ignores aerosol mass in ice-phase particles to save computation time.

c. Rate change of moments

Equations for the growth (time-rate change) of moments have three basic forms. The simplest form is associated with the initiation processes, such as activation, nucleation, or ice multiplication. For these processes, the fundamental formulas usually provide either the rate change in the number or mass mixing ratios (i.e., M_0 and M_3) of the new particle. Still needed is the rate change of M_2 , which is obtained from the rate change of M_0 and M_3 through the following relationship:

$$\frac{dM_2}{dt} = \left[\left(\frac{\alpha_{\text{int}}^2 + 3\alpha_{\text{int}} + 2}{\alpha_{\text{int}}^2 + 6\alpha_{\text{int}} + 9} \right) \frac{dM_0}{dt} \frac{dM_3^2}{dt} \right]^{1/3}, \quad (8)$$

where α_{int} is the specified initial spectral dispersion, with a value of 3 for PI nucleation or ice multiplication, or 2996 [corresponding to the maximum value of q at 0.999 in Eq. (4a), and close to a monodisperse distribution] coherent for RI initiation from the mean-size of rimed crystals.

The second form is the vapor diffusion growth processes, for which the rate change in moments can be generally written as

$$\begin{aligned} \frac{dM_j}{dt} &= \int K_j n(D) dD = \int \frac{dD^j}{dt} n(D) dD \\ &= \int \frac{2j}{\pi} D^{j-3} \frac{dV}{dt} n(D) dD, \end{aligned} \quad (9)$$

where K_j is the growth kernel for the j th moment, $V = (\pi/6)D_3$ is the particle volume, and dV/dt can be obtained from the diffusion growth equation. Note that the diffusion growth process does not affect the number mixing ratio (except sublimation), and one can easily show that $dM_0/dt = 0$ in Eq. (9). The rate change in the two associated properties can be written as the following:

$$\frac{dQ}{dt} = \frac{\pi \rho_{\text{ap}}}{6} \frac{dM_3}{dt}, \quad (10)$$

$$\begin{aligned} \frac{dF}{dt} &= \int \frac{d(\phi D^3)}{dt} n(D) dD \\ &= \int D^3 \frac{d\phi}{dt} n(D) dD + \int \phi \frac{dD^3}{dt} n(D) dD. \end{aligned} \quad (11)$$

The solution to Eq. (10) is straightforward, while the solution to Eq. (11) depends on the hydrometeor types. For PI crystals, CT16 applied the parameterization of CL94a, which relates shape change to volume change via a fundamental parameter of k , described as follows:

$$\frac{d \ln \phi}{dt} = k \frac{d \ln V}{dt}, \quad (12)$$

where k is a parameter that controls the primary growth habit and is mainly a function of temperature [see Eq. (5) in CT16]. The secondary growth habit, such as hollows and notches, is considered by using a temperature- and supersaturation-dependent ρ_{ap} in Eq. (10). With Eq. (12), CT16 derived solutions for Eq. (11) (cf. supplemental section D). For SA that is without habit consideration, one can simply set $d \ln \phi = 0$ (or $k = 0$) in Eq. (12) so the aspect ratio is constant during vapor diffusion processes.

The third form of growth processes are collisions between two particles of either the same or different hydrometeor categories. The rate change of the j th moments during collision processes can be expressed as

$$\frac{dM_{j,x}}{dt} = - \iint D_x^j K_{\text{agg}} n(D_x) n(D_y) dD_x dD_y, \quad (13a)$$

$$\frac{dM_{j,y}}{dt} = - \iint D_y^j K_{\text{agg}} n(D_x) n(D_y) dD_x dD_y, \quad (13b)$$

$$\frac{dM_{j,z}}{dt} = + \iint D_z^j K_{\text{agg}} n(D_x) n(D_y) dD_x dD_y, \quad (13c)$$

where x , y , and z indicate the contributor, the collector, and the coagulated particle, respectively; and K_{agg} is the coagulation kernel. Similarly, the rate change in shape moment can be written as follows:

$$\frac{dF_x}{dt} = - \iint \phi_x D_x^3 K_{\text{agg}} n(D_x) n(D_y) dD_x dD_y, \quad (14a)$$

$$\frac{dF_y}{dt} = - \iint \phi_y D_y^3 K_{\text{agg}} n(D_x) n(D_y) dD_x dD_y, \quad (14b)$$

$$\frac{dF_z}{dt} = + \iint \phi_z D_z^3 K_{\text{agg}} n(D_x) n(D_y) dD_x dD_y. \quad (14c)$$

In the above two sets of equations, analytical solutions are difficult to obtain especially for the coagulated particle, not only because of the complicated coagulation kernel but also because of large uncertainties in the coagulated size D_z and shape ϕ_z (which will be discussed later). As a first-order approximation, the size and shape parameters are simplified by replacing them with their modal mean so that they can be taken out of the integral, such as

FIG. 2. Schematics of the aggregation geometry that applied in this study. The aggregation involves two parent particles (y collecting x). Volume overlap is allowed in this geometry.

$$\frac{dM_{j,z}}{dt} \approx \overline{D_z^j} \iint K_{\text{agg}} n(D_x) n(D_y) dD_x dD_y, \quad (15a)$$

$$\frac{dF_l}{dt} \approx \overline{\phi_l D_l^3} \iint K_{\text{agg}} n(D_x) n(D_y) dD_x dD_y, \quad (15b)$$

where $l = x, y$, or z , $\overline{D_l} = (M_{3,l}/M_{0,l})^{1/3}$, and $\overline{\phi_l D_l^3} = F_l$ is simply the shape moment of l . Then, the solution to the integral part of Eq. (15) follows the conventional bulk method. Furthermore, the mean-size approximation is also applied in calculating the coagulation kernel K_{agg} (including fall speed and collection efficiency that contained in it) (see section D in the online supplement).

Even with mean-size approximation, the parameters of D_z and shape ϕ_z need to be determined in order to solve Eqs. (13) and (14). As volume or shape is not conserved during aggregation, one cannot obtain the aggregated size and shape simply from changes in parent particles. This problem is solved by applying the aggregation geometry shown in Fig. 2. For the shape of the resultant aggregate, the approach of Chen and Lamb (1994b, hereinafter CL94b) is followed to express the aggregated shape in terms of the overlapping dimensions using two specified parameters: 1) the separation ratio S , defined as the ratio of the overlapped maximum dimension to the sum of the maximum dimensions of the two aggregating particles; and 2) the crossing angle θ , defined as the angle between the major axis of the aggregated particles. According to Fig. 2, the separation ratio in the direction of long and short axes can be expressed respectively as

$$S_L = \frac{2L_L}{D_{L,y} + D_{L,x}\lambda_2}, \quad S_S = \frac{2L_S}{D_{S,y} + D_{S,x}\lambda_2}, \quad (16)$$

where L_L and L_S are the horizontal and vertical distance between the centers of particles x and y ; $D_{L,l}$ and $D_{S,l}$, respectively, are the long- and short-axis lengths of particle l ($l = x$ or y); $\lambda_2 = \sqrt{1 - \lambda_1}$ and $\lambda_1 = \lambda_{\text{max}}(1 - \rho_l/\rho_{bi})$,

where $\lambda_{\max} = \sin\theta$ (with $\theta = 45^\circ$ being the maximum crossing angle of crystal x and y); ρ_{bi} is the bulk density of ice; and ρ_l is the apparent density of particle l . The density term accounts for the higher possibility of crossing for less dense (e.g., more branches or hollows) ice crystals. The separation ratios range from 0 to 1, and the two limits represent the conditions of maximum and minimum overlap, respectively, while a random overlap should have a mean of $S = 0.5$. CL94b applied $S_L = 0.6$ according to observation results for the aggregation between single crystals (Kajikawa and Heymsfield 1989), likely with very small crossing angles. Due to a lack of other relevant information, we set both S_L and S_S to 0.6 for all aggregation, and include the effect of crossing angle in the form of Eq. (16). The sensitivity of the resultant aggregate shape to the value of the separation ratio will be discussed later.

With the above parameterizations, the long and short axes of the aggregated particle can be written as follows (cf. Fig. 2):

$$D_{L,z} = \frac{1}{2}[D_{L,y} + \max(D_{L,y}, D_{L,x}\lambda_2 + 2L_L)], \quad (17a)$$

$$D_{S,z} = \frac{1}{2}[D_{S,y} + \max(D_{S,y}, D_{S,x}\lambda_2 + 2L_S, D_{L,x}\lambda_1 + 2L_S)]. \quad (17b)$$

The declaration of maximum conditions is used to avoid the new dimensions becoming smaller than the original dimensions of y , which can happen when the dimension of x is very small. In addition, contribution to the length of the short axis in Eq. (17b) may come from either the short or the long axes of x depending on the crossing angle. With the long and short axes defined, the aspect ratio of the aggregated particle can be expressed as

$$\phi_z = \frac{D_{S,z}}{D_{L,z}}. \quad (18)$$

Also, according to the spheroidal shape assumption, the volume–dimension relationship of the aggregated particle can be expressed as

$$\frac{6}{\pi}V_z = D_{L,z}^2 D_{S,z} \equiv D_z^3, \quad (19)$$

where D_z is the diameter of a volume-equivalent sphere. By combining the above two equations, the shape-volume factor in Eq. (14) can be derived as

$$\phi_z D_z^3 = \frac{D_{S,z}}{D_{L,z}} D_{L,z}^2 D_{S,z} = D_{L,z} D_{S,z}^2. \quad (20)$$

The evaluation of Eq. (17) will depend on whether the long axis of the parent particles corresponds to their c axis or a axis. For prolate particles,

$$D_{L,l} = D_l \phi_l^{2/3} \quad \text{and} \quad D_{S,l} = D_l \phi_l^{-1/3}, \quad (21a)$$

whereas for planar (oblate) particles,

$$D_{L,l} = D_l \phi_l^{-1/3} \quad \text{and} \quad D_{S,l} = D_l \phi_l^{2/3}, \quad (21b)$$

where D_l is the volume-equivalent diameter of particle l . Note that the shape of SA is always oblate, but the shape of PI can be either prolate (columnar) or oblate (planar). Therefore, three types of shape aggregation may occur:

(i) prolate–prolate aggregation ($x = y = \text{prolate PI}$)

$$D_z^3 = \left[\frac{(1+S_L)}{2} (D_y \phi_y^{2/3} + \lambda_2 D_x \phi_x^{2/3}) \right]^2 \times \left[\frac{(1+S_S)}{2} (D_y \phi_y^{-1/3} + \lambda_2 D_x \phi_x^{-1/3}) \right], \quad (22a)$$

$$\phi_z D_z^3 = \left[\frac{(1+S_L)}{2} (D_y \phi_y^{2/3} + \lambda_2 D_x \phi_x^{2/3}) \right] \times \left[\frac{(1+S_S)}{2} (D_y \phi_y^{-1/3} + \lambda_2 D_x \phi_x^{-1/3}) \right]^2; \quad (22b)$$

(ii) oblate–oblate aggregation ($y = \text{SA or oblate PI}$, $x = \text{SA or oblate PI}$)

$$D_z^3 = \left[\frac{(1+S_L)}{2} (D_y \phi_y^{-1/3} + \lambda_2 D_x \phi_x^{-1/3}) \right]^2 \times \left[\frac{(1+S_S)}{2} (D_y \phi_y^{2/3} + \lambda_2 D_x \phi_x^{2/3}) \right], \quad (23a)$$

$$\phi_z D_z^3 = \left[\frac{(1+S_L)}{2} (D_y \phi_y^{-1/3} + \lambda_2 D_x \phi_x^{-1/3}) \right] \times \left[\frac{(1+S_S)}{2} (D_y \phi_y^{2/3} + \lambda_2 D_x \phi_x^{2/3}) \right]^2; \quad (23b)$$

(iii) oblate–prolate aggregation ($y = \text{SA}$, $x = \text{prolate PI}$)

$$D_z^3 = \left[\frac{(1+S_L)}{2} (D_y \phi_y^{-1/3} + \lambda_2 D_x \phi_x^{2/3}) \right]^2 \times \left[\frac{(1+S_S)}{2} (D_y \phi_y^{2/3} + \lambda_2 D_x \phi_x^{-1/3}) \right], \quad (24a)$$

$$\phi_z D_z^3 = \left[\frac{(1+S_L)}{2} (D_y \phi_y^{-1/3} + \lambda_2 D_x \phi_x^{2/3}) \right] \times \left[\frac{(1+S_S)}{2} (D_y \phi_y^{2/3} + \lambda_2 D_x \phi_x^{-1/3}) \right]^2. \quad (24b)$$

Next, the mean-size approximation is applied to simply the D_z^3 and $\phi_z D_z^3$ terms as $\bar{D}_z^3$ and $\bar{\phi}_z \bar{D}_z^3$, respectively, by

using $\overline{D}_x$, $\overline{D}_y$, $\overline{\phi}_x$, and $\overline{\phi}_y$ to replace D_x , D_y , ϕ_x , and ϕ_y in Eqs. (22)–(24). With these approximations, Eqs. (13c) and (14c) can be solved.

The rate change in mixing ratio for ice categories x and y can be determined fairly easily by combining Eqs. (10) and (13) such that $dQ_l/dt = (\pi\rho_l/6)dM_{3,l}/dt$, where $l = x$ or y , and $\rho_l = (6Q_l/\pi)M_{3,l}$, whereas for ice category z , $dQ_z/dt = -dQ_x/dt - dQ_y/dt$, based on the mass conservation principle.

d. Microphysical processes

The liquid-phase parameterizations are adopted from CL04 including the formation of raindrops and cloud drops from the collision breakup of raindrops, which were obtained by a statistical fitting of results simulated with a multimoment bin model. For the microphysical processes, the aerosol activation technique in a Lagrangian framework from Cheng et al. (2007, 2010) was used. This approach resolves maximum supersaturation by treating each grid box as an ascending or descending air parcel and calculates the changes in condensation nuclei (CN) and thermodynamics fields caused by activation and diffusional growth with smaller time steps. It means that the saturation adjustment assumption commonly applied in traditional schemes is unnecessary and that the number of activated cloud drops or raindrops can be simulated more accurately. Other microphysical processes are calculated in an Eulerian framework with a larger time step. CN is assumed to have a trimodal lognormal distribution following Whitby (1978). The cutoff size of CN to be activated into cloud drops/raindrops depends on supersaturation according to the Köhler equation; meanwhile, the prognostic mass of dry (or interstitial) CN, CN in cloud drops and CN in raindrops that have been tracked in the scheme can be used to diagnose previous cutoff size.

For the ice- and mixed-phase parameterizations, the nucleation parameterization from Meyers et al. (1992), Chen et al. (2008), Hoose et al. (2010), and DeMott et al. (2010) are implemented to choose optionally. Ice multiplication, initiated from the splintering of RI and SA during riming, is based on Hallett and Mossop (1974). The PI crystals initiated through primary and secondary productions (so-called multiplication) are assumed to be spherical, with an initial density of 910 kg m^{-3} and an initial diameter of $6\text{ }\mu\text{m}$ (cf. CL94a and CT16), and initial size spectrum spectral dispersion of $\alpha = 3$. The variation of the PI's shape and apparent density is dominated by deposition growth based on the CT16 parameterization. The initial SA aspect ratio and apparent density are determined from the self-collection among PI, and then vary according to the collision between PI and SA or SA

self-collection, as discussed earlier. Both RI and HS are still assumed to be spherical. Although Jensen et al. (2017) resolved the transition from partially rimed crystals to nearly spherical graupel, the observed aspect ratio of graupel–hail generally was 0.8 or greater (Heymsfield 1978; Straka et al. 2000). So, we ignored the shape variation of RI in the current scheme. Hence, only the density effect is considered in the calculations of fall speed and collision processes for RI and HS. Riming apparent density is based on the parameterization of Cober and List (1993). The shape and density for SA and RI (density only) are allowed to become more spherical and denser during melting through a diagnosed liquid fraction. The dry and wet growth modes of hailstones are based on the approach of CL94b with shedding raindrops in a 1-mm diameter. The fragmentation of PI, SA, and RI particles is neglected. Treatment of other microphysical processes (i.e., freezing of cloud drops and raindrops) are similar to those described in MY05b and by Morrison and Pinto (2005). More details are given in the supplement, including hydrometeors' source and sink terms, mass–dimension, area–dimension, and terminal velocity–dimension relationships for solid crystals, as well as growth kernels for diffusion, aggregation, riming, accretion, and melting mechanisms with shape consideration.

3. Idealized squall-line simulations

The National Taiwan University (NTU) multimoment bulk microphysical scheme has been implemented into the WRF Model (Skamarock et al. 2008), version 3.8.1, and tested with a standard two-dimensional idealized squall-line case, which has been frequently used to examine the performance of microphysics schemes (e.g., Morrison et al. 2009; Van Weverberg et al. 2012; Morrison and Milbrandt 2015; Song et al. 2017; Bae et al. 2019).

a. Model setup

The model is initialized with the default sounding data of Weisman and Klemp (1982, 1984), which represents a squall-line environment. The horizontal grids have 601 points in the grid spacing of 1 km, while 80 layers are applied to the vertical grids. All physics options are turned off except for the microphysical scheme to minimize interactions among physical schemes. The convection is triggered with a thermal bubble with maximum perturbation of 3 K in potential temperature centered at a height of 1.5 km. The initial CN concentration is horizontally homogeneous and decreases exponentially in the vertical with a scale height of 3.57 km, except for the lowest three sigma levels or below 850 hPa

FIG. 3. Vertical profiles of radar reflectivity for the S3M run in the first 6 h. The x axis is horizontal distance (km). The black thick solid line represents the -2 -K isotherm of perturbation potential temperature indicating the cold pool region, and the gray dotted lines are ambient temperature isopleth ($^{\circ}\text{C}$).

(cf. Cheng et al. 2007). The composition of CN is assumed to be ammonium sulfate, while the size distribution is trimodal lognormal of clean continental type as described by Whitby (1978). The primary production of ice crystals follows the implicit parameterization of DeMott et al. (2010) for deposition and condensation-freezing nucleation with a given potential ice nuclei number concentration of 400 L^{-1} (cf. Georgii and Kleinjung 1967; CL94b). Simulated radar reflectivity is derived considering the variations of the size spectrum, and the influences of bulk shape and apparent density are included through the parameterization of Ryzhkov et al. (2011).

b. Control run cloud structures

1) PRECIPITATION EVOLUTION

The evolution of the convection system is presented first with the radar reflectivity distribution from the control (CTRL) (S3M) run as shown in Fig. 3. Triggered with an initial thermal perturbation around the center of

the domain (a horizontal distance of 300 km), the convective system developed a core of high radar reflectivity reaching 50 dBZ in the first hour of simulation. The storm expanded and became increasingly asymmetric due to the vertical wind shear imposed. At 6 h, the squall-line system reached a quasi-steady state together with a distinct leading edge of convection rainband (>40 dBZ), which shifted eastward from the initial location to around 400 km in horizontal distance, and a trailing stratiform anvil that extended westward for more than 200 km.

Figure 4 shows the Hovmöller diagram of surface precipitation and column-maximum radar reflectivity. One can see a narrow band of convective core ($>25\text{ mm h}^{-1}$ and >45 dBZ), which remained stationary for the first 2 h, then traveled 100 km eastward for the next 4 h. This result is quite similar to that of Bae et al. (2019) but different from that of Morrison et al. (2009), who showed an eastward movement of the convective core less than an hour after the start of the simulation. To the west of the convective core is the trailing stratiform zone with much weaker precipitation intensity ($<10\text{ mm h}^{-1}$) and radar

FIG. 4. Hovmöller diagrams for the variation of (a) surface precipitating rate and (b) column-maximum radar reflectivity through time (ordinate) and space (abscissa) from the S3M run.

reflectivity ($<35 \text{ dBZ}$). The area of stratiform precipitation is significantly narrower than those obtained by Morrison et al. (2009) and Bae et al. (2019), while the associated radar reflectivities are smaller by about 10 dBZ. A comparison of simulations using the Morrison scheme (Morrison et al. 2009) and Milbrandt–Yau two-moment scheme (MY05a,b) are presented in the appendix.

2) HYDROMETEOR PROFILES

For simplicity, the mature squall line at 6 h will be focused on in the following analyses. The vertical profiles in Figs. 5m–r show that cloud drops and raindrops are principally absent in the stratiform cloud above the melting level, except for a few places of embedded convections. The mass concentration reached several grams per cubic meter in the convective core but is below 1 g m^{-3} in the stratiform anvil; meanwhile, the number concentration reached several hundred particles per cubic centimeter in the convective region and a few tens of particles per cubic centimeter in the stratiform anvil. The mean size of cloud drops is generally greater than $10 \mu\text{m}$ in the convective core and above $5 \mu\text{m}$ in the stratiform anvil. On the other hand, the size of raindrops may exceed 1 mm below the melting level of the convective core and become increasingly smaller getting deeper into the stratiform anvil.

The simulated PI is widely distributed over the convective core and the stratiform anvil above the 0°C level, with maxima below 1 g m^{-3} (Fig. 5a). A large number of PI is present above the -30°C level as a result of primary

nucleation mechanisms, with concentrations reaching 1000 L^{-1} above the convective core and several hundred per liter in the stratiform anvil (Fig. 5b). A secondary peak of PI number concentration on the order of 10 L^{-1} exists at the levels between -3° and -10°C (about 4.2 to 5.3 km in altitude), corresponding to the secondary ice production (i.e., the Hallett–Mossop mechanism). These low-level PIs, especially in the stratiform anvil, can have mean sizes reaching several hundred micrometers (Fig. 5c), which are far above the size threshold for cloud ice imposed in traditional bulk schemes. So, it is also possible that some of the PIs here may be contributed from ice falling aloft because of their significant fall speeds.

SA and RI are also widely distributed in the mixed-phase zone, although the amount (especially the mass) is higher toward the lower levels (Figs. 5d–i). Also, there is more RI in the convective zones, while more SA exists in the stratiform anvil. Some penetration below the 0°C level can be observed for SA and RI, and they exist as wet snow and wet graupel in our scheme. The mass concentrations of SA and RI are generally a few tenths of a gram per cubic meter. A broad area of the mixed-phase zone contains up to a few tens of particles per liter for SA and RI, except at the upper levels of the convective core and stratiform anvil where a high number of SA exceeding 100 L^{-1} were formed due to the high number of PI. The mean size of SA is generally greater than 0.6 mm at the lower part of the mixed-phase zone and may reach above 1 mm in certain parts of the stratiform anvil (Fig. 5f). RI has a similar size range, except in the convective zone where it can reach

FIG. 5. Vertical profiles of the (left) mass concentration, (center) number concentration, and (right) bulk-mean diameter for the six hydrometeors [(top to bottom) pristine ice, aggregates, rimed ice, hail, cloud droplets, and raindrops, respectively], as simulated in the S3M run at 6 h. Note that the prognostic variables Q and N have been converted from mixing ratios to concentrations.

FIG. 6. Vertical profiles of the (left) aspect ratio, (center) apparent density, and (right) bulk volume-weighted fall speed for (top) pristine ice, (middle) snow aggregate, and (bottom) rimed ice for the S3M run at 6 h. The imposed lower limit for SA aspect ratio is 0.001.

millimeter sizes (Fig. 5i). The mean sizes of RI in the convective core can be even bigger at levels below the 0°C level due to the preferential melting of the smaller RI. A similar phenomenon can be found for both SA and RI at the base of the trailing anvil cloud due to preferential sublimation of smaller particles.

This simulation produced a moderate amount of HS in the convective core and, to a lesser extent, in the convective cells embedded in the stratiform anvil, with maximum water content reaching over 1 g m^{-3} , whereas the number concentration is generally below 1 L^{-1} (Figs. 5j,k). The mean size of HS is generally a few millimeters only (Fig. 5l), which is not much bigger than RI; such limited growth after conversion from RI is due to insufficient lifting by the updraft such that the HS to fall quickly to the melting zone.

3) ICE PARTICLE SHAPE AND DENSITY

Our scheme places special emphasis on ice particle shape and density, and Fig. 6 shows that these parameters

do vary significantly. The bulk aspect ratio (volume-weighted mean; defined as F/M_3) of PI exhibited an alternating pattern of planar–columnar–planar–columnar shape variation with temperature, which generally agrees with the ice crystal primary habit diagram of Nakaya (1954). However, one can also see exceptions, such as between 250 and 370 km, where the planar (columnar) PI from above the -10°C (-20°C) level are large enough (cf. Fig. 5c) to fall and intrude to the columnar (planar) regime below; as the columns are becoming minority, the bulk shape tends to be planar (Milbrandt and Morrison 2016). This reflects the fact that our scheme considers the memory of shape. The bulk aspect ratios of SA are mostly between 0.6 and 0.8 (Fig. 6d). There are two main areas of lower aspect ratios. This first is at east end and west end of the cloud top, where the SA was recently formed from the self-aggregation of aspherical PI (cf. Fig. 6a); the other is in the central part of the cloud, where a large amount of SA (Fig. 5d)

self-aggregated to form large ($>600\mu\text{m}$) SA (cf. Fig. 5f). The area of high SA aspect ratios (>0.8) is mainly associated with wet SAs located just below the 0°C level.

The simulated apparent density of PI is mostly above 900kgm^{-3} ; but it may reduce to 850kgm^{-3} in patchy areas between -10° and -20°C , which indicates the development of secondary growth habits in the high-vapor-density zone. Another region of relatively low PI density occurred along the lower edge of the trailing stratiform cloud where the PIs were sublimating. Here, the apparent density of SA is more varied (Fig. 6e). It is generally higher near the cloud top, where they were just initiated from the aggregation of high-density PI, or below the 0°C level, where partial melting caused the SA to collapse. Fluffy SA, with apparent densities as low as 100kgm^{-3} , is generally associated with low aspect ratios (cf. Fig. 6d) and large bulk sizes (cf. Fig. 5f). The tendency of decreasing density with increasing diameter is consistent with previous observations of snow properties (e.g., Passarelli and Srivastava 1979; Brandes et al. 2007). The density of RI is the highest in the convective core (due to either the wet growth process or the high impact velocity that is associated with large sizes) and in the lower part of the stratiform cloud (due to partial melting). In the middle section of the stratiform cloud deck, RI's density is generally between 100 and 300kgm^{-3} , indicating dry growth dominant and low impact velocity. Near the top of the anvils, the apparent density of RI is somewhat higher, mainly because the RI was formed recently from high-density PI.

4) ICE PARTICLE FALL SPEED

The volume-weighted bulk fall speed of ice particles (Figs. 6c,f,h) exhibits a similar pattern as their mean sizes, with the exception below the melting level where wet SA and RI obtained higher fall speeds. The fall speeds of PI and SA are generally below 3ms^{-1} , whereas RI at the lower part of the convective core may reach 7ms^{-1} due to its larger mean size and higher density. In general, the overall trends of decreasing with altitude and from the convective core to stratiform anvil in the simulated diameter, density, and fall speed are consistent with the microphysical characteristic of mid-latitude squall lines (Houze et al. 1989).

The calculations of the fall speed of solid-phase hydrometeors follow the theoretical parameterization of MH05, which considered the effects of crystal shape and density in addition to the commonly known size effect. Figure 7a shows that, for a given size, the fall speed of PI generally decreases with increasing asphericity. The overlap between data from different shape

ranges is mainly due to variations in PI's apparent density (cf. Fig. 6b). The bulk fall speed of SA shows larger spreads because SA has large variations in both apparent density and shape. As the apparent density and shape of SA are somewhat related (low densities tend to be associated with low aspect ratios; cf. Figs. 6d,e), only the fall speed dependence on apparent density is demonstrated in Fig. 7b. Obviously, larger fall speeds are associated with higher densities. The overlap between data from different density ranges is contributed mainly from the shape variation. The highest fall speeds (at bulk-mean sizes of approximately 0.6mm) are not associated with the largest SAs but rather those shrunk due to partial melting (i.e., wet SA). RI showed a similar dependence of bulk fall speed on density (Fig. 7c). RI's fall speed clearly separated into two distinct populations, and this is related to the two modes of growth by riming—the dry growth that produces low-density RI (mostly in the stratiform anvil) and the wet growth that produces high-density RI (mostly in the convective region). As the riming rate and density both depend on fall speed, fall speed and riming density are coupled to each other in our scheme. Figure 7c also shows the bulk fall speed of HS to be slightly larger than that of the high-density RI.

Note that each moment of a hydrometeor category has its own fall speed. Bulk fall speed of the j th moment (hereafter simply called the j th-moment fall speed) is defined as $v_j \equiv \int D^j v(D) n(D) dD / \int D^j n(D) dD$. Other things being equal, the bulk fall speed should be larger for a higher-order moment unless the size spectrum is monodispersed. Figure 7d shows that PI's fall speed is slightly larger in the third moment than in the zeroth moment, indicating that the size spectrum of PI should be quite narrow. By contrast, the fall speeds of SA and RI vary more strongly with the order of moments (Figs. 7e,f).

The main difference between the 3M and 2M representations is in the spectral dispersion α in Eq. (1), which is a variable in the former but held constant (usually zero) in the latter. The addition of the spectral dispersion term also influences the “slope” (λ) term [cf. Eq. (4b)]. So, an understanding of the variability and behavior of α and λ may help justify the 3M (or variable- α) approach. Furthermore, if α varies systematically, then an alternative 2M approach using diagnosed α may be feasible. Note that a large α indicates a narrow size distribution (especially at the small-size end), which is usually associated with the condensation growth, the conversion to other hydrometeors with size preference, or the conversion from uniform-sized hydrometeors, whereas smaller α tends to associate with collision broadening or mixing of particles of assorted sizes that formed at different times or locations.

FIG. 7. Relationship between the bulk fall speed (ordinate) and the bulk volume-weighted mean size (abscissa) of (left) pristine ice, (center) snow aggregate, and (right) rimmed ice plus hailstones according to the S3M simulation at 4–6 h for (a)–(c) volume-weighted (i.e., third moment) and (d)–(f) number-weighted (i.e., zeroth moment) fall speeds. The bulk fall speeds demonstrated here have been adjusted to a fixed atmospheric condition of 0°C and 850 hPa to remove the influence of air density. The gray and black solid dots in (c) and (f) are empirical power-law fall speeds at 0°C and 850 hPa for lump graupel (Locatelli and Hobbs 1974) and hail (Matson and Huggins 1980), respectively, whereas the gray dots in (b) and (e) are for unrimmed aggregates (Locatelli and Hobbs 1974).

Figure 8 shows that PI's α value is highly variable; it largely stays in the range of 3–6 but may reach several tens in patches of the cloud, especially where both Q_{PI} and N_{PI} are high (cf. Figs. 5a,b). Note that, although the patterns of Q_{PI} and N_{PI} look smoother individually, they do not match each other exactly; therefore, the patterns of α and λ look patchier than these prognostic variables. Because the growth of each hydrometeor is influenced by many microphysical processes, which have different effects on α , the overall (domain average) correlation between α and mean particle size is rather weak, with correlation coefficients R generally within ± 0.16 for all ice-phase hydrometeors. The values of α and λ for cloud drops and raindrops are diagnosed according to Eq. (4), and they are generally high (up to several tens) in the convective zone but low ($\alpha < 3$) in most of the stratiform anvil (Fig. 8i). Such a pattern is similar to that of the mean cloud drop size (Fig. 5o). The value of α for raindrops is generally smaller than 3 (Fig. 8k). Again, the overall correlation between α and particle size is still rather weak for cloud drops ($R = 0.15$) and raindrops ($R = -0.15$).

From Eq. (4b) one can see that $\lambda = (\alpha + 3)/D_e$, where $D_e \equiv M_3/M_2$ is the effective diameter, which also equals $[\Gamma(\alpha + 4)/\Gamma(\alpha + 1)]^{1/3}/D_{vm}$, where $D_{vm} \equiv (M_3/M_0)^{1/3}$ is the volume-mean diameter. This means that, while other factors are fixed, λ should be higher for a smaller size or a larger α . Therefore, one can see a positive correlation between λ and α in Fig. 8, which ranges from 0.66 for PI to 0.93 for HS. A certain degree of positive dependence of λ on size can be observed for all hydrometeors except cloud drops and HS. For cloud drops, there is an inverse dependence of λ on size because of the inverse dependence of condensation growth rate on size (i.e., $dD/dt \propto 1/D$), which makes the size distribution narrower (and thus larger α and λ) as the droplets get larger. Yet, PI also grows by condensation (vapor deposition) but does not show an inverse dependence of λ on size. One explanation is that PI's vapor deposition growth is also affected by its aspherical shape, which tends to be more aspherical as PI gets larger; therefore, the stronger shape effect for larger PI tends to offset the inverse dependence of size growth rate on size. Another possible cause is that PI is continuously produced over

FIG. 8. Vertical cross sections of the (left) spectral index and (right) slope parameter of the six hydrometeor categories [(top to bottom) pristine ice, aggregates, rimed ice, hail, cloud droplets, and raindrops, respectively] from the S3M run at 6 h.

time (whereas cloud drops are generally initiated in a short duration near the cloud base), and the continuous supply of small PI tends to broaden the size spectrum. On the other hand, the inverse dependence of λ on size for HS is likely due to its preferential conversion from the largest RIs, as well as a limited riming growth after formation to broaden the size spectrum.

4. Sensitivity simulations

a. Shape and moment effects

The consideration of ice particle shape and density, as well as the use of triple-moment size distribution, allows a detailed description of ice particle fall speed. Two sensitivity simulations were designed to examine these influences, which are named O3M and O2M, whereas the control run, named S3M, is the simulation that was presented earlier. The prefix “S” or “O,” respectively, means with or without the particle shape variation, whereas the suffix “3M” or “2M,” respectively, indicates the three- or two-moment ($\alpha = 0$) approach.

The effect of shape and moment treatments on a hydrometeor’s microphysical properties are rather complicated, so we simplify the discussion by focusing on the vertical profiles of the volume-weighted mean size [$\bar{D} \equiv (M_3/M_0)^{1/3}$] using the contoured frequency by altitude diagrams (CFAD) as shown in Fig. 9. In general, significant differences can result from either the shape or the 3M considerations. Contrasting O3M with S3M, one can see that the spherical assumption does not noticeably affect the overall mean size of PI (101 vs 102 μm), but this is only because the slower vapor deposition growth (when spherical) is compensated by the higher fall speeds, which leads to stronger ventilation effect as well as deeper penetration (the readers may focus on the 0.6% isopleth) into the levels with more abundant liquid water to support the Wegener–Bergeron–Findeisen (WBF) conversion. These effects are amplified when the 2M treatment is applied, as evidenced by the O2M results; this is because the 2M approach tends to cause a broader size spectrum and thus greater volume-weighted size or fall speed for PI. The effect of shape on mean size and vertical penetration is more obvious for SA, partly because SA inherits some shape and density properties from PI (especially the larger ones that are more likely to aggregate) and partly due to the shape effect on fall speed and aggregation efficiency. RI’s CFAD is less affected by the shape effect because our scheme does not consider its shape variation. But one can still see a slight increase in the overall mean size of RI by contrasting O3M (overall $\bar{D} = 613 \mu\text{m}$) to S3M (overall

$\bar{D} = 593 \mu\text{m}$) results. Although RI is always spherical in S3M and O3M, the differences seen here are mainly resulted from the initialization of RI by riming on PI or SA. The riming process depends on the collection cross-section area, collection efficiency, and fall speed, all of which depend on the particle shape. Similar to what happened to PI and SA, the 2M treatment caused a reduction in the overall mean size for RI. However, the 2M treatment also produced more frequent large RI (see the frequencies at $\bar{D} > 1.5 \text{ mm}$) at heights below 5 km. This reflects the fact that, in the O2M run, RI particles at the upper levels are smaller mainly because they were formed from smaller PI and SA. Nevertheless, the 2M scheme results in higher bulk fall speed, such that larger RI can grow and penetrate to the lower levels. HS behaves similarly to RI, so the details are skipped here. As can be seen from Fig. 10, the effect of moment representation on fall speeds is even more pronounced than on mean size.

The vertical profile of ice-phase hydrometeors eventually influences the amount of precipitation on the ground. Figure 11 shows that the control run (i.e., S3M) produced relatively steady peak precipitation (generally between 20 and 40 mm h^{-1}) in the convective core at the later stage (e.g., after 3 h) of the storm evolution; but in the O3M simulation, the peak precipitation exhibited somewhat more pronounced fluctuation from <20 to $>50 \text{ mm h}^{-1}$ in the peak intensities. The O2M simulation produced less frequent $>50 \text{ mm h}^{-1}$ intensities than in the control run and a wider stratiform rain region. Overall, both the shape and moment treatments have a significant influence on the microphysical structure of the squall-line system.

Another set of tests were performed on the moment representation of individual hydrometeor categories. The S3M-IS2 applied 3M to PI and SA only, while the S3M-GH2 applied 3M to RI and HS only. As shown in Fig. 12, the general CFAD patterns are similar, but the details can be quite different. For example, the overall mean sizes can be reduced by 36%, 48%, and 8% for PI, SA, and RI/HS, respectively. Also, by changing the RI/HS scheme from 3M to 2M, the SA mean size can also be altered by 14%, apparently due to SA and RI interactions. Furthermore, the SM3-GH2 run produced a spatial pattern of surface precipitation (figure not shown) close to that from the O2M run shown (cf. Fig. 11c). This indicates that the cause of changes in surface precipitation when changing from 3M to 2M ice scheme is mainly from the calculation of the RI/HS process.

Earlier, it was mentioned that precipitation in the stratiform region (cf. Fig. 4) is weaker and more narrowly distributed than that simulated by Morrison et al. (2009) and Bae et al. (2019). The shape and moment treatments discussed above could contribute to such differences. However, other factors may also be responsible.

FIG. 9. Normalized contoured frequency by altitude diagram for bulk volume-weighted mean diameter of (top) pristine ice, (middle) snow aggregate, and (bottom) rimed ice derived from the (left) S3M, (center) O3M, and (right) O2M simulations during 4–6 h. The domain-averaged bulk diameters are listed at the top right of each panel.

For example, the treatment of aerosol–cloud interactions is quite different among the schemes, but this factor is difficult to analyze due to the inherent structural differences in these schemes. To test the effect of fall speed parameterization, two simulations were added: S3M- v_r and S3M- v_x , where the postfix v_r or v_x indicates that traditional

power-law formula (which relates fall speed to diameter) was used to calculate the fall speed of raindrops (v_r) or all hydrometeor particles (v_x), respectively. Figure 11 shows that using the power-law formula for raindrops (S3M- v_r), the peak precipitation intensity in the convective region becomes weaker while the stratiform precipitation

FIG. 10. As in Fig. 9, but for bulk volume-weighted fall speed.

area becomes somewhat wider. When extending the power-law-type calculation to all hydrometeors (S3M- v_x), the widening of the stratiform-rain region is even more pronounced. Also note that the eastward traveling speed of the convective core is somewhat slower in the S3M- v_x run, reaching only 350 km as compared to 380–400 km in other simulations. Note that nonlinear feedbacks may exist between the gravitational sedimentation and other

microphysical processes due to different parameterization methods, and the discussions above may be valid only for this particular case.

b. Initial spectral dispersion and aggregate separation ratio

In the following, additional sensitivity tests were conducted to examine the uncertainties associated with

FIG. 11. Hövmoller diagrams demonstrating the sensitivity of precipitation distributions to various microphysical treatments. The ordinate is the time of simulation, and the abscissa is the location (km) on the model domain. The color scale indicates the surface precipitation intensity (mm h^{-1}). (a) S3M is the control run with full physics, (b) O3M turns off the shape variation, and (c) O2M further assumes that the spectral index is fixed (i.e., a two-moment treatment); (d) S3M- v_r and (e) S3M- v_x are the same as the control run, except that the fall speeds of raindrops (v_r) and all hydrometeors (v_x), respectively, are calculated using the simplified power-law formulas.

the assumed values of two parameters in our method, including the α value (for deriving M_2) assigned to the newly formed PI (from either primary or secondary production processes), and the value of short-axis separation ratio S_s in the aggregation calculation. The original simulation S3M applied an initial spectral dispersion of $\alpha_{\text{int}} = 3$ following the setup of CT16, whereas, in the sensitivity test S3M- $\alpha 0$, α_{int} is set to zero to mimic the size spectrum that would be assumed in traditional 2M schemes. For the separation ratio of the short axis, the original setup is $S_s = 0.6$, whereas in the sensitivity tests S3M-S7 and S3M-S5 the value is assumed to be $S_s = 0.7$ and 0.5 , respectively.

The initial spectral dispersion for PI actually has minimal effect on PI's number and mass concentrations but has a more obvious influence on SA because of the dependence of the aggregation rate on PI's size and thus the width (or α) of PI's size distribution. The frequency distribution in Fig. 13 shows that the S3M- $\alpha 0$ simulation produced overall smaller, denser and more spherical SA particles as compared to S3M, with overall mean size

reduced from 0.35 to 0.29 mm. The mean aspect ratio increased from approximately 0.639 to 0.672, and the mean apparent density increased from 243 to 339 kg m^{-3} . A likely cause is that the zero spectral dispersion forces that the size spectrum was required to maintain many small particles, as illustrated in Fig. 1. Because the variations in bulk shape and density of SA during initiation and accretion processes are highly dependent on the size of PI, one can expect that change in the spectral dispersion will accumulate in all properties of SA during subsequent growth. Note that the aspect ratio of SA tends toward a value between 0.5 and 0.7 as they grow larger, and that this asymptotical value is close to the range of 0.6–0.8 for large SA, as indicated by the calculation of Westbrook et al. (2004) and the observations of Korolev and Isaac (2003). The range of SA's apparent density is generally consistent with the observations of snow by Passarelli and Srivastava (1979). Other properties, such as the rainfall rate and radar reflectivity, do not change significantly when $\alpha_{\text{int}} = 0$ is applied to simulate this squall-line system. However, we suspect that the

FIG. 12. As in Fig. 9, but for simulations (left) S3M, (center) S3M-IS2, and (right) S3M-GH2.

differences may become more obvious in ice-phase dominant clouds, such as snowstorms.

One of the major uncertainties in simulating the aggregation process is the separation ratio shown in Eq. (16), especially in the short dimension. From Fig. 14 one can see that this factor has a strong influence on the overall shape of SA. The overall (domain average during 4–6 h) bulk aspect ratio changed from 0.639 in the S3M run to 0.772 and 0.492 in the

S3M-S7 and S3M-S5 runs, respectively. As the SA grow larger, their bulk aspect ratio tends toward a large value of approximately 0.8 for $S_s = 0.7$ and approximately 0.4 for $S_s = 0.5$. These are quite different from the 0.5–0.7 in the control run. So, setting both S_s and S_L to 0.6 tends to yield optimal results that agree with the observed aspect ratio of 0.6–0.8 for large SA. Yet, differences in radar reflectivity and precipitation intensity among the S3M, S3M-S7, and S3M-S5

FIG. 13. Frequency distribution of the snow aggregate (top) bulk aspect ratio and (bottom) bulk density as a function of bulk diameter from the (left) S3M and (right) S3M- $\alpha 0$ simulations during the time period of 4–6 h. The color scale indicate the percentage of occurrence within each size range of 0.075 mm and aspect ratio range of 0.05 or density range of 50 kg m⁻³. The overall mean aspect ratio and apparent density are listed at the top right of each panel.

runs are not significant and thus will not be elaborated further.

We also made an arbitrary assumption on the mass redistribution when converting PI or SA to RI during riming. We took equal amounts of mass from the collector and the rime mass. Two sensitivity runs were conducted, one with a mass fraction from the collector halved and the other doubled. In general, the results are rather similar (figures ignored), indicating that the initial mass fraction is not a sensitive parameter.

5. Discussion

Another microphysical scheme that also adopted the method of CL94a to simulate the evolution of crystal habit was developed by Harrington et al. (2013), which was later improved by Jensen et al. (2017) for a more detailed treatment of ice-phase hydrometeors. Here, we address major differences between their and our approaches. First, Harrington et al. (2013) simulated PI's shape by tracking the a axis and c axis independently; Jensen et al. (2017) further separated PI

FIG. 14. As in Figs. 13a and 13b, but for simulations (a) S3M, (b) S3M-S7, and (c) S3M-S5.

into two individual categories of planar and columnar PI (as represented by prolate and oblate spheroids) and allowed different habits to coexist. By contrast, the NTU scheme keeps track of the bulk (volume weighted) aspect ratio of PI, not the axis lengths. Although only one bulk aspect ratio was allowed at a given time and space, CT16 showed that the bulk aspect ratio approach can confidently capture the overall shape and mass evolution for a mixture of planar and columnar ice crystals as simulated with a bin model. Note that in Harrington et al. (2013) the individual axes lengths could be used to diagnose particle volume, whereas mixing ratios of spheroid volume and a volumelike variable are tracked independently in ISHMAEL (Jensen et al. 2017) and our schemes. In this sense, three schemes used the same number of variables to simulate PI.

Another distinction in the schemes is that Jensen et al. (2017) allowed PI to evolve into densely rimed particles without converting into other ice categories. The separation of solid-phase hydrometeor type (e.g., oblate, prolate, graupel, densely rimed ice, unrimed branched ice, and cloud ice) is diagnosed from assumed criteria in general ice properties such as aspect ratio, density, and fall speed. Their third ice species—the aggregates—is described with prognostic mass and number, while the maximum dimension is derived by assuming constant shape and density. In the NTU scheme, the separation of ice-phase hydrometeors is based on formation mechanisms; therefore, PI can only grow by vapor deposition, while SA can grow by aggregation and vapor deposition, and RI by riming and vapor deposition. Lightly to moderately rimed cloud ice may still maintain a degree of asphericity, which may influence the

vapor deposition and riming rates; this factor can be treated in the schemes of P3 and ISHMEAL but not in our scheme as our RI is still assumed to be spherical. A future version of our scheme may be possible to include shape evolution of RI using a similar treatment for tracking the shape of SA during aggregation.

The other merit of our scheme is the addition of a third moment M_2 , which enabled a more accurate description of the evolution of the size spectrum for all ice-phase hydrometeors. Of course, the additional moment (as well as other prognostic properties such as bulk shape and volume) inevitably puts a burden on computation and thus may hinder the application of the scheme in forecasting models.

One of the key simplifications made in our scheme is the mean-size approximation applied in Eqs. (15) and (22)–(24). The error associated with such an approximation depends on the growth kernel's order of dependence on size (cf. Chen et al. 2013). Assuming the kernel is to the j th order (i.e., $K = aD^j$), the rate change in the k th moment and its mean-size approximation, respectively, can be expressed as

$$\frac{dM_k}{dt} = \int aD^j D^k n(D) dD = aM_{j+k}, \quad (25)$$

$$\frac{d\bar{M}_k}{dt} = a\bar{D}^j \int n(D) dD = a\bar{D}^j M_0, \quad (26)$$

where $\bar{D}$ is the n th-moment-weighted mean size defined as $\bar{D} \equiv (M_n/M_0)^{1/n}$. The error associated with the mean-size approximation in (26) can be expressed in terms of its ratio to Eq. (25). Figure 15 shows that the error (deviation from unity) is larger when α is

FIG. 15. Error associated with the mean-size approximation. The ordinate is the ratio of the mean-size approximation $\widetilde{dM}_k/dt$ to the true solution dM_k/dt of the k th-moment rate change; the abscissa is the spectral index α ; and $i = j + k$ is the order of moment-weighted growth kernel in Eq. (25).

smaller or when n deviates further from i . An effective way to minimize the error associated with the mean-size approximation is to select a value for n that is closest to the order of the growth kernel. That is our reason for us to use volume-weighted mean size to simplify the terms D_x^3 , D_y^3 , and D_z^3 in Eqs. (15) and (22)–(24).

6. Conclusions

The NTU multimoment bulk microphysical scheme was developed and integrated into the WRF Model to simulate the evolution of crystal shape and density through various microphysical processes. Major new treatments in the scheme include 1) applying the triple-moment (the zeroth, second, and third moments) closure method to better describe the size distribution of ice-phase hydrometeors; 2) redefining the solid-phase hydrometeors according to the formation mechanisms, which are pristine ice, snow aggregate, rimed ice, and hailstones; 3) permitting the crystal shape and apparent density to evolve with gradual adjustment according to growth conditions; and 4) coupling the bulk fall speed of frozen particles to ice shape and density.

The idealized 2D simulations using NTU scheme captured important features of the squall-line system, such as the eastward movement of the convective core, the gradual development of the stratiform anvil

region, and the transition of dominance of pristine ice to snow (aggregates) and graupel (rimed ice) toward the lower part of the cloud. These features are generally similar to those of past studies, with the main exception being that our scheme produced weaker precipitation from the stratiform anvil region. The NTU scheme produced large spatial and temporal variations in ice particle shape and density. An alternating pattern in the vertical distribution of pristine ice's shape was developed in accordance with the conventional knowledge of primary growth habit's temperature variation. Fluffy and large snowflakes appeared in the lower part of the cloud deck, with aspect ratios approaching the observed values of 0.6–0.8. The apparent density of dry snow aggregate and rimed ice in the range of 50–400 and 50–600 kg m^{−3}, respectively, were also reasonably simulated. Also simulated were changes in density and the shape of large solid particles to become denser and more spherical while melting below the 0°C level. The bulk fall speeds were shown to vary with ice-phase hydrometeors' aspect ratio, diameter, and apparent density. Large variations in the size distribution parameters α and λ were also simulated, indicating that the addition of a third moment allows for a more flexible evolution of the size distribution.

Several sensitivity tests showed that the treatment of ice particle shape, the inclusion of a third moment, and the parameterization of fall speeds all have a significant influence on the squall line's microphysical structure and surface precipitation amounts. The shape treatment can enhance diffusional growth (cf. Figs. 9a,b) but reduces the fall speed of pristine ice crystals (cf. Figs. 7a,d), whereas the triple-moment treatment yields less of the largest and smallest particles, and produces overall lower bulk fall speeds (cf. Figs. 7a,d), which also lead to weaker ventilation effect (cf. Figs. 9h,i), compared to the double-moment approach. Both treatments tend to cause weaker precipitation on the ground. In contrast to the traditional power-law parameterization, a more detailed calculation that considers particle size, density and shape tends to produce smaller fall speeds and consequently weaker surface precipitation. All these factors contribute to the weaker precipitation in the stratiform region compared to earlier studies of the same idealized case.

Although the representations of ice microphysical properties (i.e., variable shape and density) and size spectrum evolution (i.e., triple-moment) have been improved with the NTU scheme, some uncertainties remain. For example, the information of ice particle shape and density has yet to be included in the

already oversimplified ice–ice and ice–drop collision efficiencies. Also, the growth kernel for the aggregation process needs to be simplified using a mean-size approximation in order to obtain an analytical solution for the conversion rate. More accurate treatments for obtaining bulk solutions for such processes may be feasible in the future. Rimed ice is assumed to be spherical in our current scheme, but studies have shown that the asphericity of rimed ice (and graupel) may have many microphysical consequences (cf. List and Schemenauer 1971) similar to those for snow aggregates. Our current scheme also cannot effectively describe polycrystals such as bullet rosettes, side planes, or chained aggregates, which may behave quite differently from the pristine ice or snow aggregate that we defined. A more comprehensive description of shape and density for all ice-phase hydrometeors may be necessary for future cloud models because of their importance not only in microphysics but also radiative processes as well as in polarimetric radar simulations. Some recent developments of microphysical parameterizations, such as ice multiplication by collision fragmentation (Phillips et al. 2017) or bulk liquid fraction of ice particles (Cholette et al. 2019), are certainly worthy of inclusion in our scheme if the influence of particle shape and density can be determined.

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APPENDIX

Comparison with the MOR and MY2 schemes

The idealized 2D squall-line simulation was also conducted using the microphysical options “MOR” (Morrison et al. 2009) and “MY2” (MY05a, b), both of which are double-moment schemes. Note that the default setting of graupel category in MOR scheme has been switched to the property of hail. Below is a brief discussion of the comparisons.

Figure A1 shows that the NTU scheme (S3M) produced much narrower stratiform precipitation than the other two schemes; however, the vertically projected maximum radar reflectivity in Figure A2 shows a much broader distribution. Figure A3 shows that the radar reflectivity from NTU was weaker below 4 km and outside the convective region comparing those from the other two schemes. These results indicate that the NTU scheme did produce a sizeable trailing anvil that contains a significant amount of precipitation particles, but the precipitation particles simply cannot reach the ground (mainly due to smaller fall speed as discussed in the main text). Note that the patterns of radar reflectivity look quite different when we included the shape and density effects in the radar simulator (Figs. A3d,e vs Figs. A3a,b).

The vertical profiles of hydrometeor mass concentration in Figure A4 shows that the NTU produced more PI but less SA/RI in terms of mass concentration. Part of this is due to the different definition of ice-phase hydrometeors, because our PI may exceed the conventional size threshold for snow. This also explains why the peak of PI mixing ratio in our scheme is located at a significantly lower altitude

FIG. A1. Hövöller diagrams of precipitation intensity (mm h^{-1}) from the three microphysical schemes: (a) NTU, (b) MOR, and (c) MY2.

FIG. A2. Hövmøller diagrams of vertically projected maximum total equivalent radar reflectivity (dBZ) for the (a) NTU, (b) MOR, and (c) MY2 schemes with a dielectric constant fixed at 0.224. (d),(e) As in (a) and (b), respectively, except that the effects of ice property (i.e., shape and density) on scattering amplitudes are considered in the radar simulator. In (d), the reflectivity was calculated using the same code as that provided with the MOR scheme.

FIG. A3. As in Fig. A2, but for the vertical profiles of total equivalent radar reflectivity at 6 h.

idealized 2D squall line domain-averaged-profiles of mass mixing ratio

FIG. A4. Vertical profiles of domain-average mass concentration for various hydrometeors from the three microphysical schemes. Note that the prognostic variables Q have been converted from mass mixing ratio to mass concentrations.

than in the other two schemes. The less SA and RI in our scheme is mainly due to the difference in fall speed calculation such that our SA and RI fall faster to lower levels (cf. Fig. 7), which may also explain why NTU scheme produced more rainwater but not in the expense of cloud water (the NTU scheme retained significantly more cloud water than the MY2 and MOR schemes do).

Although the hydrometeors' mass contents may be quite different, the patterns of vertical variation in mass partitioning among the three ice-phase hydrometeor categories (RI and HS are combined) from the three schemes are generally similar (Fig. A5). Furthermore, the vertical profiles of ice-phase hydrometeors' number concentrations are actually quite similar (except for hail) among the three schemes especially at heights below about 8 km

FIG. A5. Vertical profiles of domain-averaged ice mass partition ratio among the three ice-phase hydrometeors from the (left) NTU, (center) MOR, and (right) MY2 schemes.

FIG. A6. Vertical profiles of domain-averaged number concentration for various hydrometeors from the three microphysical schemes. Note that the prognostic variables N have been converted from number mixing ratio to number concentration.

(Fig. A6), indicating that the initiation processes for each ice-phase category are similar among the three schemes.

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