The Spectral Ice Habit Prediction System (SHIPS). Part I: Model Description and Simulation of the Vapor Deposition Process

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(Manuscript received 30 January 2006, in final form 16 October 2006)

ABSTRACT

This paper describes the Spectral Ice Habit Prediction System (SHIPS), which represents a continuous-property approach to microphysics simulation in an Eulerian cloud-resolving model (CRM). A two-moment hybrid-bin method is adopted to predict the solid hydrometeor distribution, where the distribution is divided into the mass bins with a simple mass distribution inside each bin. Each bin is characterized by a single representative ice crystal habit and the type of solid hydrometeor. These characteristics are diagnosed based on a series of particle property variables (PPVs) of solid hydrometeors that reflect the history of microphysical processes and the mixing between bins and air parcels in space. Thus, SHIPS allows solid hydrometeors to evolve characteristics and size distribution based on their movement through a cloud.

SHIPS was installed into the University of Wisconsin-Nonhydrostatic Modeling System (UW-NMS) and tested for ice nucleation and vapor deposition processes. Two-dimensional idealized simulations were employed to simulate a winter orographic storm observed during the second Improvement of Microphysical Parameterization through Observational Verification Experiment (IMPROVE-2) campaign. The simulated vertical distributions of ice crystal habits showed that the dynamic advection of dendrites produces wider dendritic growth region than local atmospheric conditions suggest. SHIPS showed the sensitivities of the habit distribution in the low- and midlevel to the upper-level growth mode \((T < -20°C)\) of ice crystals through the sedimentation. Comparison of the results to aircraft observations casts doubt on the role of the columnar growth mode \((T < -20°C)\) traditionally thought to be dominant in the literature. The results demonstrated how the complexity of the vapor deposition growth of ice crystals, including dendrites and capped columns, in varying temperature and moisture lead to particular observed habits.

1. Introduction

Cloud-resolving models (CRMs) of the earth atmosphere have been developed over the past four decades to explicitly simulate microphysical processes in order to 1) predict their impact on the modeled thermodynamics and dynamics and 2) to simulate the cloud structure and attendant precipitation. Nevertheless, the underlying microphysical processes are still only partially understood, and formulated with a combination of basic theory, empirically derived relationships, and educated approximations to fill the many gaps in knowledge.

Microphysics schemes applied to multidimensional Eulerian CRMs can be classified into two paradigms: (i) bin (or spectral) schemes (e.g., Takahashi 1976; Farley and Orville 1986; Kogan 1991; Ovtchinnikov and Kogan 2000), and (ii) bulk microphysics schemes (e.g., Lin et al. 1983; Thompson et al. 2004). Both schemes require categorization of solid hydrometeors (or ice particles) to be predicted. The differences arise primarily from methods to approximate size distributions of hydrometeors. Size variations are discretized explicitly into multiple size or mass “bins” with the bin model approach. This approach is the least restrictive on developing arbitrary size distributions, but requires a large number of size bins to represent a complete size spectrum. For this reason, the bin approach has not been feasible for three-dimensional CRMs, except when applied to a limited number of categories of hydrometeors. Recently, Lynn et al. (2005) implemented a fast version of the spectral (bin) microphysics model (SBM Fast) in a 3D Eulerian mesoscale model,
the fifth-generation Pennsylvania State University—National Center for Atmospheric Research (PSU—NCAR) Mesoscale Model (MM5) to simulate a convective cloud system. They have defined three categories of solid hydrometeors: plate, dendrite, and column category, and used larger mass bins of the categories for aggregates, graupels, and hail particles.

The “bulk” approach to explicit microphysics prediction, first proposed by Kessler (1969), approximates the typically bimodal distribution of liquid hydrometeors by assuming that there are two separate categories of liquid droplets, one precipitating (rain) and one too small to precipitate (cloud droplets). It is further assumed that each category is distributed in a simple statistical distribution characterized by one—two moments that can be predicted or assumed based on empirical studies. The bulk technique was extended to the ice phase (e.g., Koenig and Murray 1976; Orville and Kopp 1977; Cotton et al. 1982; Lin et al. 1983) by also dividing ice particles into several distinct categories including cloud ice category (analogous to cloud droplets) and precipitating ice categories typically called snow, and graupels (analogous to rain). In addition to the classic bulk size distribution assumptions, each category requires the assumption of specific mass—diameter relationship, mass—velocity relationship, bulk density of the ice particles, or diagnosis of a geometry of ice particles (or ice crystal habit) to formulate microphysical behavior and tendencies. Therefore, the category to which a particular ice particle belongs is critical to its evolution and movement, how it interacts with other categories, and how it behaves radiatively in a CRM. The properties of ice particles at a given time suggest the past dynamical and microphysical processes experienced by the particles. Inversely, a series of processes or particle history and local environment at a given time determines the properties. In other words, ice particles indicate dynamical and microphysical memory whereas liquid hydrometeors show little. However, the particle property is predefined in traditional bulk and bin approaches by categories, and the growth history is retained only in form of concentration and mass content of the predefined categories. Thus, the accuracy of the traditional bulk or bin approaches might be increased by implementing more and more specialized categories, having more predicted parameters for each category. Having more categories leads to more possible routes of mass content and concentration among the categories, and introduces more arbitrary decisions between them. In a practical sense, conventional bulk and bin approaches for solid hydrometeors are a “discrete-property approach.”

In this paper, we develop the Spectral Ice Habit Prediction System (SHIPS) that evolves the property of ice particles by diagnosing particle growth history for each bin of one mass spectrum of ice particles. By introducing the variables that define properties of ice particles for each bin, the categorizations of ice particles are not necessary and so the complicated, arbitrary transfer links among categories are unnecessary. Rather than converting mass between categories, SHIPS mixes properties. Hence through growth and transport, ice crystal habit and structure evolve. SHIPS is a “continuous-property approach” by allowing solid hydrometeors to evolve the properties continuously.

SHIPS is one component of Advanced Microphysics Prediction System (AMPS). The other components of AMPS are the Aerosol Prediction System (APS) and the Spectral Liquid Prediction System (SLIPS). This study uses University of Wisconsin-Nonhydrostatic Modeling System (UW-NMS; Tripoli 1992) as the CRM. It has been modified to maximize the efficiency of AMPS, but AMPS is built to function with the dynamics of any CRM.

This paper is the first in a three-part series—Part I: description of SHIPS infrastructure, and verification of simulation of ice nucleation and vapor deposition processes; Part II: development of a general model for vapor deposition process that incorporates polycrystals; and Part III: description and verification of aggregation and riming processes. Section 2 will describe the underlying framework of SHIPS. Section 3 will discuss implementation of SHIPS into the Eulerian UW-NMS CRM. Then, in section 4, the formulation of the vapor deposition process and terminal velocity that reflect crystal habit will be described. Section 5 briefly describes the setups of UW-NMS and AMPS to simulate a winter orographic storm during the second Improvement of Microphysical Parameterization through Observational Verification Experiment (IMPROVE-2) field experiment and also presents the experiment design. Results of the model simulations will be evaluated and compared to observations of IMPROVE-2 in section 6, and finally, conclusions will be drawn in section 7.

2. Spectral Habit Ice Prediction System (SHIPS)

SHIPS is designed to retain growth history as conserved particle characteristics that can move throughout the cloud and mix with other particles of different characteristics. Rather than assigning ice particles to predefined categories such as cloud ice, pristine crystals, or graupel, we define a distinguishable group of hydrometeors contained within an air parcel only by 1) concentration, 2) mass content, and 3) series of evolved characteristics that reflect the growth history [particle
property variables [PPVs)]. PPVs can include the amount of mass of a hydrometeor accumulated from a microphysical process, lengths along the crystallographic axes of an ice crystal, circumscribing volume, electric charge, mass of liquid coating, and so on. The number of PPVs depends on the complexity of the scheme desired.

In addition to the ability to predict ice particles of differing physical characteristics, SHIPS is designed to predict multimodal distributions with moderate computation. This research adopted a two-moment bin method with a subdistribution assumed over a bin.

An important assumption of the SHIPS framework is the implicit mass sorting assumption, which states that different species of solid hydrometeors within a single air parcel, defined by a set of growth parameters, are naturally sorted by mass. Hence, for now, each mass bin can only represent a single set of mean habit characteristics and mean type of solid hydrometeors that are distinguished by mass, number concentration, and PPVs predicted for the bin. The limitation is softened, however, by the fact that the mass–habit relationship for a bin can vary over time and between grid cells as a result of microphysical evolution and transport. The representation of a single habit and single type for a mass bin also means that simulations with SHIPS are somewhat sensitive to the number of bins used. The number of bins corresponds to maximum number of habits and types that can be diagnosed over the mass spectrum, and the range of mass occupied by one bin, therefore one habit, gets larger when less numbers of bins are used. The dependence of growth processes and sedimentation on habits leads to a difference in the resulting concentration and mass fields of hydrometeors.

a. Hybrid-bin method

The mass-bin scheme of SHIPS, which this study uses in an Eulerian dynamic model, is based on the multi-component hybrid-bin method proposed and demonstrated in Lagrangian parcel model by Chen and Lamb (1994a, hereafter CL1). It was adopted for its simplicity and flexibility for defining collision kernels. CL1 described the spectrum of concentration of ice particles by three independent variables: water mass, solute mass, and aspect ratio of hydrometeors. The axis of each variable was divided into bins: 45 water mass bins, 20 solute mass bins, and 11 aspect ratio bins. The hybrid-bin method conserves two moments of subdistribution along the axis of each independent variable. To reduce computational cost, we simply describe the spectrum as a function of total mass of a hydrometeor. Hence, predicted two moments are the number concentration and mass content of a bin.

The subdistribution in a bin is described by piecewise linear distribution (see CL1 for a more detailed description):

$$n(m) = n_0 + k(m - m_0),$$  \(1\)

where the number of particles per mass and volume of air \(n(m)\) is described in terms of mass of the particle \(m\), \(m_0\) is the midpoint of mass-bin boundaries, and \(n_0\) is the concentration per mass at \(m_0\). Let \(m_1\) and \(m_2\) be the left and right mass boundaries of the \(b^{th}\) bin. See appendix C for a description of the symbols used in this paper. This study defines the mass boundaries as

$$m_b^1 = m_b^{b - 1} = k_b m_1 m_2^{b - 1},$$  \(2\)

where \(k_{b_0}^{bb}\) is an arbitrary constant. Then, concentration and mass content predicted for the \(b^{th}\) bin are defined by

$$N^b = \int_{m_1}^{m_2} n(m) \, dm,$$  \(3\)

$$\varrho^b = \int_{m_1}^{m_2} mn(m) \, dm.$$  \(4\)

The two moments of the subdistribution of the bin are related to the two parameters of the linear distribution:

$$n_0 = \frac{N^b}{m_2 - m_1},$$  \(5\)

$$k = \frac{12(\varrho^b - m_0 n^b)}{(m_2 - m_1)^3}.$$  \(6\)

The hybrid-bin method of CL1 calculates the increase (or decrease) of concentration and mass content for each bin after the microphysical growth processes are computed. The new concentration \(N^b\) and mass content \(\varrho^b\) defines a shifted bin with the two shifted-bin boundaries. The shifted-bin boundaries are allowed to be inside of a mass bin in order to ensure the positivity of \(n(m)\) (see CL1 for a detailed discussion). From the two new moments and shifted-bin boundaries, two parameters of the linear distribution in the shifted bin are obtained from Eqs. (5) and (6). Then, particles inside the shifted bin are transferred back into the bins defined by original bin boundaries [see Eq. (2)] finally, tendency of mass content and concentration for

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1 This paper defines “aspect ratio” as the ratio of the semiminor axis length to the semimajor axis length of a spheroid, while “axis ratio” is defined as the ratio of lengths along the crystallographic axes of an ice crystal.
the $b$th bin is calculated by subtracting the original mass content and concentration from the newly obtained mass content and concentration.

As the mass content and concentration are moved between bins, PPVs are also mixed weighted by concentration. This results in a mixed structural evolution in a given bin since the flux of mass content and concentration from neighboring bins influence the mean habit evolution in a given bin. The following section describes PPVs that are added to the CL1 hybrid-bin model for the SHIPS application.

**b. Particle property variables (PPVs)**

We define the **representative hydrometeor** of a bin as a particle whose mass is equal to the mean mass of the bin $m$:

$$m = \frac{\varrho^b}{N^b}. \quad (7)$$

SHIPS retrieves the properties of the representative hydrometeor in a bin through PPVs that reflect the history of dynamical mixing and local microphysical processes. SHIPS considers the following types of PPVs: (i) mass content components, (ii) length variable components, (iii) volume variable components, and (iv) aerosol mass content components. Figure 1 shows the schematic of SHIPS where the ice spectrum is divided into five mass bins. The formulation of continuity equations to predict PPVs in the Eulerian dynamic framework of UW-NMS CRM will be given in section 3.

1) **Mass content components**

The mass of the hydrometeor in a bin consists of four mass components: ice crystal mass $m_I$, aggregate mass component $m_A$, rime mass component $m_R$, and liquid mass component $m_L$. The sources of these components are the microphysical processes affecting the bin, that is to say, ice crystal mass $m_I$ is
produced by the vapor deposition process onto ice crystals, aggregate mass $m_A$ by the aggregation process, rime mass $m_R$ by the riming process, and liquid mass $m_W$ by the melting process. The mass components add up to mass of a hydrometeor:

$$m = m_I + m_A + m_R + m_W,$$

which is valid for any hydrometeor with mass $m$ in a bin as well as for the representative hydrometeor with mass $\bar{m}$.

It is clear that the mass components $m_I$, $m_A$, $m_R$, and $m_W$ are conservative variables as the mass of a hydrometeor. Naturally, quantities of the mass components integrated over the subdistribution are transferred between bins and grid cells. The implicit mass sorting assumption implies that the ratio of each mass component to the mass of a hydrometeor is fixed over the mass range defined by the bin boundaries; hydrometeors in a bin have the same type. Therefore, the mass content components $\varrho^{b}$, $\varrho^{a}$, $\varrho^{c}$, and $\varrho^{k}$ are proportional to the total mass content $\varrho$. Note that the proportionality of the mass content components change over time, space, and bin number. The mass content components also add up to the total mass content of the bin:

$$\varrho = \varrho^{b} + \varrho^{a} + \varrho^{c} + \varrho^{k}.$$  

In this paper, we will ignore $\varrho^{k}$, and focus on $\varrho^{b}$, $\varrho^{a}$, and $\varrho^{c}$. SHIPS predicts $\varrho^{a}$ and $\varrho^{c}$ in addition to $\varrho^{b}$, and then $\varrho^{a}$ is diagnosed from the above equation.

### 2) LENGTH VARIABLE COMPONENTS

This paper considers sixfold symmetric (hexagonal) ice crystals for the representation of ice crystals in simulated clouds. SHIPS retrieves three lengths along two crystallographic directions of a hexagonal ice crystal for the representative hydrometeor. One can add more lengths if necessary. The conceptual geometry of the hexagonal ice crystal is defined by three independent lengths $a$, $c$, and $d$ corresponding to the $a$ axis, $c$ axis, and dendritic arms (see Fig. 3a). Mass of the hexagonal crystal model is related to the lengths as

$$m = 3\sqrt{3}a^3(1 - \psi)(1 + \psi)a^3\rho^a,$$

where $\phi = ca$ and $\psi = da$ are the axis ratios, and $\rho^a$ is the bulk density of the hexagonal crystal model. The hexagonal crystal model is used to obtain the geometrical properties of ice crystals defined by Bohm (1989), which are necessary to calculate terminal velocity as discussed later. For each hydrometeor, the bulk crystal density $\rho_c$ is defined through mass–length relationships:

$$m_I = k_I(1 + 4\phi^2a^3\rho_c^a),$$

$$m_A = k_A(1 + \phi^{-2}c^3\rho_c^a),$$

$$m_R = k_R(1 + 4\phi^2d^3\rho_c^a),$$

where the volume of a sphere circumscribing the ice crystal is used ($k_s = 4\pi/3$). The bulk crystal density corresponds to the effective density defined for ice particles in Heymsfield et al. (2002).

Additional PPVs needed to retrieve the geometry of ice crystals include the concentration weighted cubic $a$-axis length, $c$-axis length, and dendritic arm lengths, $\ell_{a}^c$, $\ell_{c}^a$, and $\ell_d^c$ (or denoted by $\ell_l^a$ for $l$-axis length). To define these PPVs, constant $\rho_c$, $\phi$, and $\psi$ over mass in a bin were assumed, which stems from the implicit mass sorting assumption. Then, the mass–length relationships, Eqs. (11)–(13), are used to integrate cubic lengths weighted by concentration over the mass for each growth axis length. Therefore, $\ell_{a}^c(l = a, c, d)$ are proportional to the ice crystal mass content component, $\varrho^a$. Each length of the representative hydrometeor of mean mass $\bar{m}$ is retrieved simply by $l = \sqrt[3]{\ell_{a}^c l / \bar{m}}$ ($l = a, c, d$).

To retain the growth history of ice crystals along the various crystallographic axes of growth, it was initially considered important to predict the mass deposited along each axis instead of the length variables and then use the mass continuity equation to represent the mixing of different kind of particles in the Eulerian dynamic model. However, it was determined that the mass deposited along each axis alone did not uniquely characterize the geometry of a crystal. It was found that the axis growth history was better characterized by predicting axis-length variables together with total mass of a particle. The validity of mixing $\ell_{a}^c$ between mass bins and grid cells is discussed in appendix A.

### 3) VOLUME VARIABLE COMPONENTS

In addition to mass content components and length components, solid hydrometeors can be characterized by volume variable components that can be also defined and predicted based on microphysical process. One such volume quantity predicted in this study is the sphere volume that circumscribes one solid hydrometeor, $V_{sc}$. The volume is related to the total mass of a particle with the bulk sphere density

$$m = \rho_s V_{sc}.$$

For the case where ice particles are pristine ice crystals or rimed crystals, $\rho_s = \rho_c$. The volume variable component was determined to be necessary in order to diagnose the bulk sphere density and semiaxis lengths of aggregates and graupels.
that are categorized based on mass content components. One can also diagnose the type of solid hydrometeors as the category of ice crystals. In this way, the type of the representative hydrometeor is diagnosed using length-variable components as shown in Fig. 2.

**4) Aerosol Mass Content Components**

In the earth atmosphere solid hydrometeors form on aerosols or form by freezing supercooled liquid hydrometeors that are originally formed on aerosols. SHIPS keeps track of total mass \( m_{\text{api}} \) and soluble mass \( m_{\text{aps}} \) of the aerosols. Insoluble mass of the aerosols \( m_{\text{api}} \) are diagnosed as \( m_{\text{api}} = m_{\text{apt}} - m_{\text{aps}} \). In the same way as the mass content components, the ratio of each aerosol mass content component to the total mass content of the hydrometeors in a bin is assumed to be constant. Therefore, the aerosol mass content components \( \rho^b_{\text{aps}} \) and \( \rho^b_{\text{api}} \) transferred by microphysics processes between bins are easily calculated from the transferred mass content \( \rho^b \) with the ratio in a shifted bin.

**c. Diagnosis of habit and type**

From the predicted PPVs one can diagnose the type and habit of solid hydrometeors. This study defines the “type” of solid hydrometeors as the category of ice crystals based on physical processes that formed it (e.g., pristine crystal, aggregates, or graupels). This study defines “habit” as particular crystallographic feature of an ice crystal (Pruppacher and Klett 1997; e.g., plates, columns, dendrites, etc.). Note that categorization of solid hydrometeors itself is not necessary for SHIPS microphysics simulation. However, categorization aids in verification since observations are often classified into traditional forms found in the Magono–Lee classification (Magono and Lee 1966).

This research diagnoses types of solid hydrometeors based on mass content components as shown in Fig. 2.

Graupels are diagnosed if the bin has more mass content produced by the riming process than any other processes. Bins with mass content dominantly produced by aggregation are diagnosed as aggregates. If the mass content produced by riming is less than the aggregation mass content in a bin, then the particle type is considered to be rimed aggregates. In the same way, a bin containing mass content largely produced by vapor deposition are diagnosed to certain pristine crystals, and those with some riming mass content but less than mass content by vapor deposition are regarded as rimed crystals.

The diagnosis of solid hydrometeor types is robust because it depends only on the microphysical processes that the air parcel experiences. However, in the in situ observation the mass estimation by each process is somewhat more challenging. Riming mass could be estimated through chemical concentration on solid hydrometeors (Borys et al. 2003; Chen and Lamb 1999). Distinction between rimed aggregates and graupel crystals would be the most difficult among them.

The habit of ice crystals is diagnosed using length-variable components as in Fig. 3b. It basically means that crystals with \( \phi < 1 \) with \( \psi \leq \frac{1}{2} \) (\( \psi > \frac{1}{2} \)) are considered as plates (dendrites) and those with \( \phi > 1 \) as columnar crystals.

**d. Outputs and possible applications**

The predicted outputs from SHIPS are concentration, mass content, and PPVs for each bin of the mass spectrum. For ice crystals, the lengths along growth axes are available. Once aggregation starts, those lengths represent the average lengths of ice crystals within the aggregate. This will be described in a subsequent paper. The bulk density, aspect ratio, and maximum dimensions of aggregates, rimed aggregates, or graupels are diagnosed from the predicted concentra-
tion, mass content, and circumscribing volume. One can attain a sense of particle history by examining the PPVs formed in each bin. Trajectories of each bin can be formed, providing an estimate of particle origins.

The crystal habit information, maximum dimension, aspect ratio, bulk density, and liquid water mass of solid hydrometeors are useful in the radiative transfer calculation. Employing the distribution of PPVs across mass bins, radiative transfer calculation can explicitly take into account particle mass, shape or length scales, density, phase structure, and so on. Diagnostic procedure can also be used to estimate secondary motions of ice particles such as tumbling behavior. Research is currently under way to evaluate the impact of these new available tools.

3. Applying the hybrid-bin method to the Eulerian dynamics framework

a. Continuity equation

The SHIPS application of the CL1 hybrid-bin model requires that the system be cast in the Eulerian framework. This requires a continuity equation be formed for each prognostic variable. The general form of the continuity equation, following Tripoli (1992) is given in tensor form as

$$\frac{\partial q_{\text{ice}}^{n,b}}{\partial t} = -\frac{1}{\rho} \frac{\partial (\rho u_i) q_{\text{ice}}^{n,b}}{\partial x_i} + \frac{q_{\text{ice}}^{n,b}}{\rho} \frac{\partial \rho u_i}{\partial x_i} + \frac{1}{\rho} \frac{\partial}{\partial x_i} \left( \rho K_{\text{H}} \frac{\partial q_{\text{ice}}^{n,b}}{\partial x_i} \right) + \frac{1}{\rho} \frac{\partial}{\partial x_i} \left( \rho \nu \frac{\partial q_{\text{ice}}^{n,b}}{\partial x_i} \right) + S_{n,b},$$

(15)

where $q_{\text{ice}}^{n,b}$ is the specific quantity of the ice parameter “$n$” in mass bin “$b$” defined as

$$q_{\text{ice}}^{n,b} = \frac{q_{\text{ice}}^{n,b}}{\rho},$$

(16)

and $\rho$ is the density of the moist air, and $q_{\text{ice}}^{n,b}$ is the quantity per unit volume of the air of the ice parameter $n$ ($n = 1, 2, \cdots, n_b$) in the $b$th ($b = 1, 2, \cdots, b_n$) mass bin. Equation (15) defines $n_b \times b_n$ as separate equations that are added to the UW-NMS CRM. Table 1 shows the corresponding prognostic variables for UW-NMS and SHIPS. We have $n_b = 10$ parameters for solid hydrometeors per bin: concentration, mass content, and PPVs explained in the previous section. The Cartesian grid unit tensor is $x_i$, and the velocity components are $u_i$. The terminal velocity of the ice parameter $n$ integrated over mass bin $b$ is given by $V_{\text{f},b}$, the eddy mixing coefficients for scalars is $K_{\text{H}}$, the high-order numerical mixing coefficient is $\nu$, and the order of the high-order filter is $l_f$.

The source term $S_{n,b}$ is defined by the SHIPS microphysics scheme and involves conversion tendencies between the ice, liquid, and vapor water species:

$$S_{n,b} = \frac{\partial q_{\text{ice}}^{n,b}}{\partial t} |_{\text{IU}} + \frac{\partial q_{\text{ice}}^{n,b}}{\partial t} |_{\text{VD}} + \frac{\partial q_{\text{ice}}^{n,b}}{\partial t} |_{\text{AG}} + \frac{\partial q_{\text{ice}}^{n,b}}{\partial t} |_{\text{RM}} + \frac{\partial q_{\text{ice}}^{n,b}}{\partial t} |_{\text{HB}} + \frac{\partial q_{\text{ice}}^{n,b}}{\partial t} |_{\text{MS}},$$

(17)

where the subscript IU denotes ice nucleation, VD is the vapor deposition process, AG is the aggregation process (collection within ice spectrum), RM is the riming process (collection between ice and liquid spectra), HB is the hydrodynamic breakup, and MS is the melting–shedding process. The microphysical computation of SHIPS uses prognostic variables that are defined for unit volume of air, whereas the dynamic part of the model requires specific quantity of the variables. Therefore, tendencies (source and sink) calculated by

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**Fig. 3.** Diagnosis of habit of the representative hydrometeor for a bin: (a) the dimension of the hexagonal crystal model and (b) the diagnosis flowchart.
the microphysics have to be divided by the density of the moist air.

This Eulerian form of the parameterization is cast in a flux conservative form, so that a budget of each parameter leaving and entering a grid cell can be maintained. A small diabatic mass source results from the elastic fluxes of the moist air mass into and out of grid cells on a small time step (Tripoli 1992). The associated lapse in conservation due to numerical approximation of the quasi-compressible closure is small and all tests show it to be entirely negligible. The numerical treatment of advection, was found to be critical to the performance of the SHIPS system. Whereas Tripoli (1992) reported good results using the sixth-order Crowley advection scheme, it was found that such a scheme was too diffusive for SHIPS and led to an artificial spreading of microphysical habits. Instead, the piecewise parabolic method (PPM) described by Colella and Woodward (1984) was adopted as the advection scheme. This scheme was found to perform superior to Crowley while maintaining accuracy in the classical nonhydrostatic model tests of mountain-wave simulation. The downside of the PPM is the nonlinearity of its operator that has the potential to move PPVs differently. This effect was noticed but seemed to be less significant than the artificial spreading with Crowley.

As mentioned earlier, flux conservative Eulerian transport results in the mass-weighted mixing of bins between grid cells. This results in the PPVs in a given bin reflecting the mean history of the same mass bin of surrounding parcels. This is both a limitation and a benefit of the approach as it does allow a local growth regime to be overwhelmed by a larger mass of ice particles entering the parcel from another location. This makes intuitive sense. On the other hand, if parcels having equal mass contents of differing particles types, the result will be a particle of mixed characteristics. We believe that this is an acceptable compromise in return for the economy of the implicit mass-sorting assumption.

b. Weighted terminal velocity and sedimentation

The sedimentation of hydrometeors in the Eulerian dynamic framework is an important process to sort hydrometeors of different masses into different altitudes. The appropriate terminal velocity for sedimentation of a prognostic variable for a bin is the one weighted according to the corresponding continuity equation. The general formulation of terminal velocity based on boundary layer theory developed by Bohm (1989) is used to obtain the terminal velocity weighted by mass and concentration within a bin. The terminal velocity \( v^b \) for the representative hydrometeor in the \( b \)th bin is calculated as

\[
v^b = \frac{N_{Re} \eta}{L_d \rho},
\]

where \( L_d \) is the characteristic length of the hydrometeor. Bohm (1989) calculates the Davies number \( X \) as

\[
X = \begin{cases} 
\frac{8 \eta g \rho}{\pi \eta^2 \max (\alpha, 1) u_{rat}^{1/3}} & \text{if } q_{rat} \leq 1, \\
\frac{8 \pi \eta^2 \max (\alpha, 1) u_{rat}^{1/3}}{\eta^2 \max (\alpha, 1) u_{rat}^{1/3}} & \text{if } q_{rat} \geq 1
\end{cases},
\]

where \( \alpha \) is the aspect ratio of hydrometeors, and \( q_{rat} \) is the area ratio (porosity) defined by the ratio of the projected (effective) area of a hydrometeor \( A_e \) to that of the circumscribing spheroid \( A_s \). The pressure drag is calculated based on aspect ratio and porosity. Reynolds number \( N_{Re} \) is calculated with the pressure drag, the Davis number and aspect ratio, and then modified by correction for transitional flow and for viscous re-
gime. As done by Mitchell (1996), the power-law relationships between $N_{ic}$ and $X$ were derived from those calculated with the formula for the hydrometeors considered in Bohn (1989). With the simple relationship and assumption of the constant aspect ratio and area ratio over a mass bin, Bohn's terminal velocity formula can be analytically integrated over each mass bin (see Mitchell and Heymsfield 2005 for theoretical approach).

The sedimentation of prognostic variables (i.e., mass content, concentration, and PPVs) with differently weighted terminal velocity can affect the property of representative hydrometeors. Having differently weighted terminal velocity for mass content and concentration leads to the sorting of hydrometeors within a bin. This leads to the shift of the mean mass where the representative hydrometeor of a bin is defined. Note that each specific PPV $q_{ic}^{n,b}$ has differently weighted terminal velocity $V_{ic}^{n,b}$ (Table 1). All mass content components have the same mass-weighted terminal velocity $V_{ic}$ as that of the total mass. This is because the ratios of the mass content components to the total mass content are assumed to be constant. Therefore, the type of solid hydrometeors that is diagnosed with the ratios of mass components is not affected by the sedimentation. Length components and volume components are assumed to have concentration-weighted terminal velocity $V_{ic}$, for each bin because those are related to each particle rather than mass. Similarly, the diagnosed habit is not affected by sedimentation because the aspect ratios are assumed to be constant within a bin. Since the mean mass of a bin is affected by the sedimentation, the representative hydrometeor of the bin may have a longer or shorter length than before.

4. Modeling dependence of depositional growth and terminal velocity on ice crystal habits

This section describes and discusses the methods to simulate vapor depositional growth and terminal velocity for continuously changing geometry (or habit) of ice crystals. Formulation of ice nucleation and the melting-shedding processes used in this study are described in appendix B. The ice nucleation processes include deposition-condensation nucleation, contact-freezing nucleation, and immersion-freezing nucleation. The melting-shedding process model estimates meltwater mass based on the steady state of the heat budget.

a. Vapor deposition process

This research uses the parameterization of vapor depositional growth of ice crystals developed by Chen and Lamb (1994b, hereafter CL2). It assumes the spheroidal ice crystal to calculate the mass, volume, and length growth. The core assumption of the process is the mass distribution hypothesis by CL2:

$$\frac{dc}{da} = \Gamma(T) \frac{c}{a^2},$$

where $\Gamma(T)$ is the inherent growth ratio that reflects current atmospheric condition onto ice crystals. The axis ratio $c/a$ indicates the history of the ice crystal. This hypothesis is important because it gives the ratio of $c$-axis to $a$-axis growth rate, and it can be used in varying ambient temperature. Based on the hypothesis, the changes of $a$- and $c$-axis lengths of a falling ice crystal under ambient temperature $T$ are linked to the change of the mass of ice particle [see Eqs. (41)–(44) of CL2]. This study calculates the mass growth of a hydrometeor having mean mass of the bin $\delta m$ by

$$\delta m = 4\pi C(a, c)G(T, p)f_ia^2s_d\delta t,$$

where $C(a, c)$ is the capacitance of the spheroid with $a$- and $c$-axis lengths, $G(T, p)$ is the thermodynamic function (see Pruppacher and Klett 1997), $f_i$ is the ventilation coefficient, $f_{m}$ is the mass-transfer correction factor for kinetic process, $s_d$ is the supersaturation over ice, and $\delta t$ is the time step.

CL2 gives the growth rate of $a$- and $c$-axis lengths of a spheroidal ice crystal. This study attempts to break the $a$-axis length into length of the inner hexagonal crystal and dendritic length extending from the vertex of the hexagonal crystal as the following. We define conditions to grow dendritic arms $d$ as

1) The diameter of hexagonal plate is more than 20 $\mu$m: $a_h > 10$ $\mu$m;
2) $-16^\circ C \leq T \leq -12^\circ C$, and liquid hydrometeors exist or saturated over water; and
3) dendritic arm $d > 10$ $\mu$m.

The main condition on the diameter of the hexagonal part is speculated based on ground observation of Auer and Veal (1970), which shows the existence of dendritic ice crystals with a diameter as small as 50 $\mu$m. The first condition on environmental temperature and moisture is well known in the literature based on laboratory experiments (e.g., Kobayashi 1961), and this is the dendritic growth regime. However, the second one is a hypothesis: the dendritic arms continue to grow even in plate or column growth region once they are initiated in a dendritic zone. It is intuitively speculated that the dendritic arms grow due to higher ventilation effect around the tip of arms.

The mass content of a shifted bin for the $b$th bin $q^b = q^b + \delta q$ is calculated by $\delta q = N^b\delta m$. Using the
linear distribution corresponding to $N^0 = N^h$ and $\rho^0$, and $\phi^0$, the mass content and concentration are transferred into the bins defined with original mass boundaries as described by CL1. We can calculate the mass content components transferred into original bins using the ratio of each component to the total mass content in the shifted bin. For vapor deposition, the change of mass content $\delta \rho$ is added only to the ice crystal mass content component.

The concentration weighted cubic length $\ell^c_{l} = [a \cdot (a, c, d)]$ transferred to the original bins from the shifted bin can be calculated as following. The $a$- and $c$-axis length in a shifted bin $a' = a + \delta a$ and $c' = c + \delta c$ are calculated, using $\delta a$ and $\delta c$ from Eqs. (41)–(44) of CL2. Only if one of the above conditions for dendritic growth is satisfied, $\delta d$ is set equal to $\delta a$, and the dendritic arm in the shifted bin $d' = d + \delta d$ is obtained. Then, the axis ratios $\phi = c'/a'$ and $\psi = d'/a'$, and bulk crystal density $\rho^c = \bar{m}/(2\pi \phi \psi a^3)$ for the shifted bin are obtained. Since there are mass–length relationships [Eqs. (11)–(13)], the transferred $\ell^c_{l}$ are easily calculated from the axis ratio, bulk crystal density of the shifted bin, and the ice crystal mass content transferred from the shifted bin.

In the similar way to the length components, the concentration-weighted circumscribing sphere volume $V^c_{cs}$ can be transferred back to the original bins. The volume $v^c_{cs}$ in the shifted bin is calculated as

$$v^c_{cs} = k_c [(a + \delta a)^2 + (c + \delta c)^2]^{3/2}$$

(22)

for pristine and rimed crystals. The concentration-weighted volume transferred from the shifted bin can be calculated from the bulk sphere density $\rho^c$ of the shifted bin and transferred total mass content [Eq. (14)]

As with mass content and concentration, the tendency of PPVs per volume of air by vapor deposition process for a bin is calculated by subtracting the original variables from the newly obtained variables.

b. Terminal velocity

The ice crystal habits can influence not only vapor depositional growth but also terminal velocity, which is especially important in determining the structure and life time of cloud systems with weak vertical motions such as cirrus and stratiform clouds (see, e.g., Heymsfield et al. 2002). SHIPS calculates the terminal velocity that corresponds to continuously changing mass and habits by the general formulation of Bohm (1989). As described above, the formula requires the aspect ratio, area ratio, and characteristic length of ice particles as well as the mass. Those are calculated from lengths predicted by SHIPS and geometry of the hexagonal crystal model as shown in Fig. 3. The hexagonal crystal model gives the area ratio of planar crystals with predicted lengths as

$$q_{int} = \frac{A_e}{A_c} = \frac{3\sqrt{3}/2(a - d)(a + d)}{\pi a^2}$$

$$= \frac{3\sqrt{3}(1 - \phi)(1 + \psi)}{2\pi}$$

and $q_{int} = 4/\pi$ for the columnar crystals as defined by Bohm (1989).

To illustrate the effect of changing axis ratios $\phi = c/a$ and $\psi = d/a$ in SHIPS, terminal velocity of a single ice crystal was calculated using Bohm’s equation. Given two axis ratios and mass, three axis lengths can be calculated from the mass–length relationship, Eq. (10), with $\rho^h = \rho$. The mass of the ice crystal was specified by substituting $a = 50 \ \mu m$, $\phi = 1.0$, and $\rho^h = \rho$ into Eq. (10). As shown in Fig. 4, the calculated terminal velocity changes continuously with $\phi$, and $\psi$ except for $\phi = 1$. The discontinuity is caused by switching the orientation of the crystal to the flow. The terminal velocity is smaller for columnar (planar) crystals with larger (smaller) $\phi$ and with longer dendritic arms, which is an important feature of habit.

5. Model setup and experiment design

A winter orographic snowstorm observed on 13–14 December 2001 during the IMPROVE-2 campaign was selected as a case study to evaluate SHIPS, following case 3 of the Sixth International Cloud Modeling Work-
shop in 2004 (Grabowski 2006). A significant cyclonic storm and vigorous upper-level cold-frontal rainband produced extensive and deep clouds and precipitation over the Oregon Cascades (Woods et al. 2005). The case is ideal for this study because the temperature and moisture distribution cover the whole range of laboratory-known plate growth, column growth, and dendrite growth regimes as well as relatively high predictability of the dynamics forced by topography. A two-dimensional idealized (slab symmetric) simulation is implemented with UW-NMS.

a. Dynamics

UW-NMS (Tripoli 1992) is implemented as the 2D Eulerian CRM that integrates microphysical variables predicted by SHIPS. UW-NMS features a time-split, compressible grid, leapfrog-forward model. A 1.5-level turbulence closure is employed. To limit the buildup of truncation error, the enstrophy conservative thermodynamic closure described by Tripoli (1992) is used in addition to kinetic energy and potential vorticity conservative. UW-NMS adopts a unique height coordinate system called “step topography” that uses a terrain-following variable grid spacing near the ground. The ice-liquid water potential temperature (Tripoli and Cotton 1981), specific humidity of total water, and other water species except vapor and pressure are predicted. Vapor-specific humidity, potential temperature, and temperature are diagnosed based on those predicted variables. Radiative forcing is not calculated in this simulation even though SHIPS produces detail properties of solid hydrometeors. As mentioned in section 3, the PPM (Colella and Woodward 1984) is implemented for advection of scalar variables. The horizontal resolution is 1 km, and the vertical resolution is 100 m for the lowest 20 points and then increased up to 500 m by the ratio of 1.1. The elevation of terrain along the cross section was provided by the workshop. The numerical filter and diffusion terms in Eq. (15) are turned off to study the effect of advection and sedimentation.

This study uses a time step of 10 s and diagnoses the vapor mass as total water mass subtracted by liquid and ice particle masses. Resolving supersaturation requires the time step on the order of 0.1 s, which is computationally expensive for operational use. It is assumed that hydrometeors consume the excess water by vapor deposition to maintain saturation over water after one time step. The supersaturation is calculated as the value with which the deposited vapor mass on the cloud condensation nuclei (CCN) after activation, ice nuclei (IN) after deposition-condensation nucleation, liquid, and ice particles within the time step are balanced with supersaturation production by advection from the dynamic model. The supersaturation over ice in the vapor deposition equation for ice particles was capped by the value at water saturation. It is important to note that the supersaturation diagnostics and ice nucleation are one of the most crucial processes to obtain a proper realization of the evolution of ice particles in SHIPS. The excess water produced from the dynamic model depends on the time step used. Therefore, the balancing supersaturation and, in turn, the concentration of ice crystals nucleated with Meyers et al.’s (1992) deposition-condensation nucleation parameterization (a function of supersaturation over ice) depend on the time step. The concentration of nucleated ice crystals play an important role in determining the habit and growth of the nucleated ice crystals given temperature and available vapor under vapor competition. Also, it affects subsequent deposition-condensation nucleation through the supersaturation diagnosis.

b. Microphysics

In the hybrid-bin method, this study uses 21 and 20 bins for liquid and solid mass spectral, respectively. The parameters used to define bins are listed in Table 2. The first bin of the liquid spectrum is set up to have mass boundaries that correspond to 0.2- and 20-µm diameter (activation transition group). The reason for the relatively large mass ratio of the first bin is that this study uses the time step that is larger than one typically required for supersaturation prediction, and the supersaturation is diagnosed as explained above. Therefore, with the diagnosed supersaturation the size distribution

<table>
<thead>
<tr>
<th>Phase</th>
<th>Group</th>
<th>N</th>
<th>$k_{bb}$</th>
<th>$a_{bb}$</th>
<th>Smallest mass</th>
<th>Largest mass</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid</td>
<td>Activation transition group</td>
<td>1</td>
<td>$1.0 \times 10^3$</td>
<td>1.0</td>
<td>$4.19 \times 10^{-15}$ g (0.1 μm)</td>
<td>$4.19 \times 10^{-9}$ g (10 μm)</td>
</tr>
<tr>
<td></td>
<td>Growth group</td>
<td>20</td>
<td>Varying</td>
<td>1.02</td>
<td>$4.19 \times 10^{-9}$ g (10 μm)</td>
<td>$5.24 \times 10^{-1}$ g (5 mm)</td>
</tr>
<tr>
<td>Solid</td>
<td>Deposition growth group</td>
<td>4</td>
<td>22.1</td>
<td>1.0</td>
<td>$4.19 \times 10^{-12}$ g (1 μm)</td>
<td>$1.0 \times 10^{-8}$ g (62 μm)</td>
</tr>
<tr>
<td></td>
<td>Collection growth group</td>
<td>10</td>
<td>2.51</td>
<td>1.0</td>
<td>$1.0 \times 10^{-6}$ g (62 μm)</td>
<td>$1.0 \times 10^{-3}$ g (620 μm)</td>
</tr>
<tr>
<td></td>
<td>Riming growth group</td>
<td>6</td>
<td>3.16</td>
<td>1.0</td>
<td>$1.0 \times 10^{-3}$ g (620 μm)</td>
<td>$1.0 \times 10^{-1}$ g (1.34 cm)</td>
</tr>
</tbody>
</table>
of haze particles (nonactivated droplets) and activated small cloud droplets, which range over the first bin or smaller mass, may not be captured accurately even by using the fine resolution of the bins. Following Chen and Lamb (1999), the rest of the liquid spectrum (growth group) is divided into bins by mass boundaries defined as Eq. (2) with varying ratio \( k_{bb} = a_{bb} k_{bb}^{-1} \) in order to capture collection process with higher resolution in larger mass. Similarly, in order to capture collection process of ice particles with a small number of bins, the mass spectrum was divided into three groups with each group having constant bin boundary ratio. Based on the mass range of different types of solid hydrometeors suggested by empirical mass–diameter relationships and the sensitivity test of collection process, we determined three groups: the depositional growth group, the collection growth group, and the riming growth group.

c. Initial conditions

Two categories of aerosols, CCN and IN, are set up as follows. Totally soluble sea salts are assumed for initial CCN, and the modal radius (0.133 \( \mu \text{m} \)) and standard deviation (0.210 In log of \( \mu \text{m} \)) of lognormal distribution are taken from the accumulation mode of the maritime distribution by Jaenicke (1993). The measured droplet concentration between 4 and 6 km in the altostratus cloud deck during the case study is 10–30 cm\(^{-3}\), according to Woods et al. (2005). Therefore, the CCN vertical concentration was initialized in such a way that it decreases exponentially with height from 25 cm\(^{-3}\) at 5 km to 0.5 cm\(^{-3}\) at 10.5 km. This gives 876 cm\(^{-3}\) at the sea level. The IN vertical concentration was initialized with 230 L\(^{-1}\) throughout the domain as done by CL1, and the radius of the uniform distribution was set to 1.0-\( \mu \text{m} \) radius. UW-NMS was homogeneously initialized with the sounding data at 1200 UTC of 13 December 2001 derived from a rawinsonde launched near Creswell, Oregon.

d. Experiment design

Three experiments are designed to demonstrate the habit simulation of SHIPS, to discuss the resulting advection of length PPVs, the current state of knowledge challenged by mixing of the habit in space, and the upper level growth mode of the ice crystal with the sedimentation effect. Table 3 lists the three experiments. They are set up with or without advection and sedimentation of solid hydrometeors and with two different growth regimes of ice crystals in temperature \( T < -20^\circ \text{C} \). The ice microphysical processes simulated in these experiments include ice nucleation, vapor deposition, and melting processes. Note that the aggregation and riming processes are not simulated in this study. The simulations with the aggregation and riming processes are described and discussed in Part III of the series.

We spun up the orographic storm simulation only with liquid microphysics first and after 12 h of simulation it reached the quasi-steady state. All the experiments were implemented by turning on ice microphysics from the quasi-steady state obtained with liquid microphysics only. The atmospheric conditions at the quasi-steady state are shown in Fig. 5. Figure 5a shows that the upward vertical motion has developed over the windward slope of the Cascades due to mountain waves indicated by potential temperature. The atmosphere is dried out through subsidence just downwind of the highest peak, but the strong leeside mountain wave formation causes clouds developing at high levels. Production of strong rainbands is shifted downwind, while the cloud droplets are nucleated in location of the upward vertical motion. These distributions of liquid hydrometeors correspond to the distribution of 0% supersaturation over water as shown in Fig. 5c. As soon as ice microphysics is turned on, ice crystals will take vapor from the moist air and liquid species above 2 km, which is about 0°C (Fig. 5b).

| Table 3. Summary of the experiment cases used to test SHIPS. All the cases simulate ice nucleation, vapor deposition, and melting processes. |
|---|---|---|
| Advection and sedimentation of ice particles | Inherent growth rate \( \Gamma(T) \) |
| EXP1 | Off | CL2’s columnar growth in \(-30^\circ < T < -20^\circ \text{C}\) and \( \Gamma(T) \) for \( T \leq -30^\circ \text{C} \) |
| EXP2 | On | Same as EXP1 |
| EXP3 | On | Planar growth of \( \Gamma(-3.5) \) used for \( T < -20^\circ \text{C} \) |

6. Results

a. Vapor deposition process and advection

For the first test of SHIPS, advection and sedimentation of hydrometeors were turned off and only the vapor deposition process was left on in order to isolate the nucleation and growth effects from subsequent mixing (EXP1). Figure 6 shows the horizontally averaged \( a \)-axis, \( c \)-axis, and dendritic arm lengths after 20 min of vapor deposition process. The peaks of the \( a \)-axis and \( c \)-axis lengths are on the order of \( 10^3 \mu \text{m} \), and the dendritic arms only exists in the thin layer at 5 km where the
ambient temperature satisfies the condition for dendritic arm growth. The Lagrangian simulation of falling ice crystals under water saturation at 700 hPa was performed for comparison (Fig. 7). The simulated lengths and their spatial distributions in the Eulerian dynamical model closely follow the Lagrangian one except below 2.5 km. The variability of the lengths in the lower level come from the contact-freezing nucleation of evaporatively cooled liquid hydrometeors.

For the second test, advection and sedimentation between grid cells in the Eulerian dynamical model were turned on, and the UW-NMS was run with vapor deposition and melting process (EXP2). For diagnostic purpose, the concentration-weighted lengths of three growth axes over the spectrum at each grid cell were calculated as shown in Fig. 8. After 20 min from the quasi-steady state, EXP2 produces a more spread region of dendritic arms than without advection (EXP1). This is because the dendritic arms were produced originally between 4 and 5 km, and then advected upward and downward. Once the radius of the hexagonal part and the advected dendritic arm reaches the threshold of 10 µm, it begins growing in any condition of temperature and supersaturation over ice.

The ice crystals were diagnosed by length variable components for each mass bin as shown in Fig. 3b. Figure 9 shows the concentration of diagnosed habits at each grid cell at 20 min of EXP2. The columnar crystals are dominant above 6 km because of 1) the high nucleation tendency by deposition–condensation nucleation, and 2) the columnar growth mode in $T < -20^\circ$C. In EXP1 and EXP2 the temperature range between $-30^\circ$C and $-20^\circ$C is defined as columnar growth mode, and $\Gamma = 1$ below $-30^\circ$C was assumed for growth of solid columns whose existence was known under low supersaturation (see Pruppacher and Klett 1997). The vertical distribution of low concentration of plates ($\approx 10^{-4}$ L m$^{-3}$) corresponds to the vertical motion $>1$ m s$^{-1}$ and the area of active immersion-freezing nucleation. Both deposition–condensation and immer-
sion-freezing nucleation contributed to the plates and dendrites in levels between 3 and 6 km.

For each diagnosed habit, the concentration-weighted lengths over the spectrum were calculated at each grid cell. Figure 10 shows the axis ratios calculated with the average lengths at 20 min of EXP2. The lhs of the figure shows that the flatness of predicted ice crystals ($\phi = c/a$) follows the temperature dependence of growth regime. The flat plates in the locations of height at $>8$ km and a distance between 150 and 210 km, and of height 3–6 km and a distance of 330 km were produced by evaporating the $c$-axis length more than $a$-axis length, although they have a very small concentration. The dendrites have the minimum horizontally averaged $\phi$ of 0.25 at 4 km, while the maximum horizontally averaged $\phi$ of the columnar crystals is about $\phi = 2$ at 2.5 and 5.5 km. The axis ratio $\phi$ of dendrites (columns) is larger (smaller) than Takahashi et al.’s (1991) observation at 20 min of ice crystal growth. This lack of sharpness in the axis ratio was found to come mainly from the large time step used. The right panel in Fig. 10 shows the axis ratio $\psi = d/a$ at 20 min. The simulation produced the broad-branched crystal and dendrites shown by (Fig. 10b) and (Fig. 10d) below 6 km, which roughly matches with the habits observed during the aircraft observation shown in Fig. 8 of Woods et al.

Fig. 6. Horizontally averaged axis lengths of ice crystals at 20 min of vapor deposition simulation without advection and sedimentation (EXP1). “Mean” is the horizontally averaged value, “SD” is the standard deviation, and “Max” is the maximum value.

Fig. 7. Lagrangian simulation of the $a$- and $c$-axis length under water saturation. Time is 1, 5, 10, 15, and 20 min from the left, and the circle and cross are observations by Takahashi et al. (1991).
Figure 10f indicates that even some columns have dendritic arms. In SHIPS the conceptual geometry of the capped column is assumed to be the columnar crystal with dendritic arms growing at the \( a \) axis. The aircraft observation shows capped columns, CP1a in 3–5 km, above and below the dendritic growth region (Woods et al. 2005). It is known that capped columns grow from columns after they go through the plate growth region (Hallett 1984) and Ono (1969) observed them around the dendritic growth region. However, quantitative conditions of temperature and moisture necessary for the growth of capped columns have not been investigated yet in the laboratory. There are at least seven known habits that have columnar components, plates, and dendritic features together as shown in the Magono–Lee diagram. Therefore, at this point SHIPS just uses the simple conditions for dendritic arm growth described in section 4. Quantitative laboratory study of ice crystals has to be done to validate the main and second condition of dendritic arms and the condition of capped column growth, in order to model the transitional growth of habit properly.

b. Sensitivity of the upper-level growth mode

In the previous section the 20-min simulation of vapor deposition and melting simulation (EXP2) featured a wider vertical area of dendrites and capped column due to advection. This section explores the sensitivity of the habit prediction to the growth mode in the upper level through the sedimentation effect. Figure 11a shows the concentration of ice crystals after 90 min of vapor deposition and melting processes (EXP2). It increases with height and reaches a horizontal mean of \( \approx 400 \, \text{L}^{-1} \) at 9 km. Compared with the magnitude of the concentration, the concentration tendency of all the ice nucleation processes shown in Fig. 11b are almost negligible except for the lower levels, the left boundary, and the locations of strong vertical motion. This indicates that a high concentration of ice crystals were hori-
horizontally and vertically advected and fell into lower levels. In fact, most of the ice crystals were nucleated during the first 20 min of simulation by the deposition–condensation nucleation process. After 20 min, the process was relatively insignificant due to depletion of available IN inside of the domain and moisture competition with growing ice crystals. On the other hand, immersion-freezing and contact-freezing processes kept their strength at the locations of strong vertical motion and lower levels.

As shown in Fig. 12, columnar crystals including capped columns are more abundant than plates and dendrites in terms of mass content. The reason for the dominance can be explained by the inherent growth ratio defined for \( T < -20^\circ\text{C} \) along with the high concentration of ice crystals in the upper level. Figure 13 shows the inherent growth ratio \( \Gamma \) defined in Eq. (20). EXP1 and EXP2 assume the inherent growth ratio \( \Gamma(T) = 1 \) for \( T < -30^\circ\text{C} \) and columnar growth regime for \( -30^\circ < T < -20^\circ\text{C} \). The nucleated ice crystals fell through the columnar growth region and grew to columns as they traveled downwind. Then, the high concentration of falling columns from above overwhelmed the planar crystals, which nucleated and grew into the

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**Fig. 10.** Comparison of average axis ratios at 20 min of vapor deposition simulation with advection and sedimentation (EXP2). The lhs shows the logarithm of \( \phi = c/a \) and the rhs shows \( \psi = d/a \).
dendritic growth regime \((-16^\circ \leq T \leq -12^\circ \text{C})\) and dendritic arms grew on the columnar crystals.

To clarify the sensitivity of the low- and midlevel habit distribution to the upper-level growth mode and sedimentation, we perform a simple sensitivity test (EXP3), where the planar inherent growth rate at \(T = -3.5\) was assigned to \(T < -20^\circ \text{C}\) (Fig. 13). As shown in Fig. 14, the ice crystals in the domain are mostly planar at 90 min of the vapor deposition and melting simulation. Note that the concentration and mass content of dendrites increased between 2 and 5 km over the crests of the Cascade. This is because more planar crystals in the upper level above 5.5 km or \(T < -20^\circ \text{C}\) were produced and then dendritic arms grew onto the plates falling from the above into the dendritic growth region. Figure 15 shows the simulated mass spectrum at a horizontal distance of 194 km at three neighboring grid cells in the vertical: (Fig. 15a) 4.4, (Fig. 15b) 4.0, and (Fig. 15c) 3.7 km. Plates are further diagnosed into broad-branched crystals if they have \(\frac{1}{3} \leq \psi < \frac{2}{3}\), and columns

\begin{figure}[h!]
\centering
\includegraphics[width=\textwidth]{fig11.png}
\caption{Comparison of (a) concentration of ice crystals [log 10$L^{-1}$] and (b) concentration tendency by all the ice nucleation processes [log 10$L^{-1}$ s$^{-1}$] after 90 min of vapor deposition simulation (EXP2).}
\end{figure}

\begin{figure}[h!]
\centering
\includegraphics[width=\textwidth]{fig12.png}
\caption{Comparison of mass contents for diagnosed habits after 90 min of the vapor deposition simulation (EXP2). The dotted contours are 0.01 and 0.05 (g m$^{-3}$) and the solid contours are 0.1, 0.2, and 0.3 (g m$^{-3}$).}
\end{figure}
are named as capped columns if they have $\frac{1}{3} \leq \psi$. Five points indicate the linear distribution of a bin, and the vertical line shows that the linear distribution can take on zero concentration (cm$^{-3}$ g$^{-1}$) on bin boundaries. The figure suggests that the ice crystals experience the transition of diagnosed habit at 4 km from broach-branched crystals to dendrites due to the growth of axis ratio to $\psi > \frac{1}{3}$. The similar dispersion and mode of mass spectra among the three indicate that the ice crystals have a similar growth history and lack of crystals with nucleation-size mass implies that they fell from a higher altitude.

The mass content estimated by Woods et al. (2005) based on the crystal habit and particle size distribution measurements along the flight legs ranges from 0.12 to 0.26 g m$^{-3}$ between 4.2 and 6.0 km (see Fig. 13 in Woods et al. 2005). Similarly, EXP2 and EXP3 showed an increase of mass content below 6 km over the peaks of the Cascade where the water-saturated condition was simulated in the model (Fig. 5). Also, both of EXP2 and EXP3 predicted the same order of mass content with the estimates for the altitude above 4 km where the active vapor deposition process was suggested in the observation. Note that EXP3 shows faster sedimentation of ice crystal mass than EXP2 due to the difference in calculated terminal velocity for the dominant habit. Dendritic ice crystals are associated with a second snowflake diameter maximum at $-12^\circ$ and $-17^\circ$C, and known to be important to the initiation of an aggregation process through a mechanical locking mechanism (Pruppacher and Klett 1997, p. 608). Therefore, in addition to the effect on sedimentation, the dominant distribution of broad-branched crystals and dendrites in EXP3 would lead to more efficient aggregation and
riming processes than that of columns and capped columns in EXP2.

Figure 16 shows the size spectra of solid hydrometeors constructed from linear distributions over bins at horizontal distance of 240 km and six altitudes from (Fig. 16a) 5.8 to (Fig. 16f) 1.55 km. The spectra become narrow toward the lower altitude and the mode shifts to a larger mass, which possibly indicates the sedimentation effect of larger particles and vapor depositional growth. Figures 16b,c show that dendrites, broad-branched crystals, plates, and columns coexist in one spectrum from a small mass below the dendrite growth area. Comparison with the leg-averaged size spectra shown in Fig. 12 in Woods et al. (2005) indicates that the predicted spectra have less concentration of ice particles in size larger than 0.25 mm. The discrepancy may stem from the initialization of ice crystal fields, neglect of aggregation and riming processes, and less available moisture. In reality the upper-level front brought ice crystals to the domain, which are missing in our initialization. The observation shows aggregates of dendrites below 4 km. As Woods et al. (2005) noted, the most significant increases of large size particles were associated with dendrites and their aggregates, thus, the aggregation process is certainly an important factor needed to predict the spectrum. Also, the 2D simulation does not have the advection of IN and ice crystals, the moisture convergence in the direction perpendicular to the cross section, and the vertical component of vorticity.

As shown above, the growth mode in $T < -20^\circ C$ can play a important role in simulation of orographic storms due to its high nucleation rate and subsequent sedimentation into altitude of active vapor deposition growth with dendritic growth mode. The sedimentation effect of the upper-level crystals simulated by SHIPS favors the plate growth mode for $T < -20^\circ C$, compared with the aircraft observation. Then, it can be asked: is the columnar growth regime at $T < -20^\circ C$ real? Bailey and Hallett (2004a, 2002) show that between $-20^\circ$ and $-40^\circ$ C plates and platelike polycrystals dominate the habit, and generally columns appear with low frequency. They pointed out that the use of silver or lead iodide for nucleation in past laboratory experiments resulted in the dominance of columns and thin and thick plates in the temperature range. The aircraft observation of IMPROVE-2 (Woods et al. 2005) also indicates the existence of assemblages of sectors, sideplanes, and plates above 4 km colder than $-15^\circ C$. As for $T < -40^\circ$ C, Bailey and Hallett (2004a) show the higher frequency of the observation of long columns and the formation of bullet rosettes with increases in moisture, but they also show the plate growth for the smaller ice supersaturation. Therefore, in order for SHIPS to provide further insights on the upper-level growth mode, representation of the polycrystal growth modes appears necessary. Research is currently under way to include these effects and will be presented in Part II of this paper.

7. Conclusions

SHIPS is a framework to explicitly evolve mass spectrum of solid hydrometeors, ice crystal habit, and shape
and density of solid hydrometeors in a multidimensional CRM by using basic physical principles. Mass spectrum of solid hydrometeors is divided into bins defined by mass boundaries and each bin has a linear distribution. The particle characteristics in a bin is expressed by a set of prognostic variables called particle property variables (PPVs). This study considers the mass content components, length variable components, volume variable components, and aerosol mass content components for the PPVs. PPVs are predicted based on the current atmospheric conditions and the growth history embedded in PPVs. SHIPS eliminates the need to assume the analytical distribution for the whole spectrum, particle properties, idealized category of ice particles, and conversion between those categories. The use of PPVs allows ice particles together with complex 2D or 3D flow fields to build realistic crystal habits and ice types.

This paper focuses on formulation and testing of the simulation of ice nucleation and vapor deposition processes. Explicit simulation of habit by length components showed not only the high potentials of this approach but also missing quantitative knowledge of growth conditions of ice crystals. The notable results are the following:

- The size and vertical distribution predicted by SHIPS correspond well to Lagrangian simulations at 20 min of the simulation where advection and sedimentation of ice crystals were turned off.
- The advection process in the Eulerian dynamics model made the growth region of dendrites wider.

![Size spectra of solid hydrometeors at a horizontal distance of 240 km from EXP3 and at an altitude of (a) 5.8 to (f) 1.55 km. The linear distribution of a mass bin is indicated with five points. The circles indicate plates, the squares indicate broad-branched crystals, the triangles indicate dendrites, the crosses indicate columns, and the plus symbols indicate capped columns.](image-url)
than local atmospheric condition would predict, and
revealed the importance of growth conditions of den-
dritic arms outside the dendritic regime. The col-
nar crystals with dendritic arms were diagnosed as
capped columns, but the quantitative growth condi-
tion of capped columns is not investigated yet in the
literature.

• A sensitivity test of upper-level growth mode of ice
crystal habit in $T < -20^\circ C$ indicated that proper
simulation of habit of this range of temperature is
crucial in orographic storms due to possible high ice
crystal concentration at the level (>6 km) and the
subsequent sedimentation into the altitude of active
vapor deposition with dendritic growth mode. Com-
parison of sensitivity tests with the aircraft observa-
tion cast doubt on the role of columnar growth re-
ime of hexagonal crystals defined for $-30^\circ < T <$
$-20^\circ C$ in the past literature and the definition of a
single growth mode given ambient temperature and
moisture in $T < -20^\circ C$.

Because dendrites are a key for aggregation and
hence, for the physical chain of precipitation process,
more quantitative studies of growth condition of den-
drites and capped columns must be done while varying
temperature and humidity. Prediction of the growth of
the $a$- and $c$-axis lengths in SHIPS relies on the mass
distribution hypothesis by CL2. Even though the tran-
sition of aspect ratio of ice crystals from colder to
warmer temperature are observed by Korolev and
Isaac (2003) and Bailey and Hallett (2004b), the core
assumption has to be verified quantitatively in labora-
tory under realistic scenarios of transitioning pressure,
temperature and humidity. For further realistic simula-
tion of ice crystals in $T < -20^\circ C$, length scales repre-
senting bullet rosettes and other polycrystalline habits
have to be incorporated into SHIPS. Part II of this
paper will report on the development of a general
model for vapor deposition growth that incorporates
the effects of polycrystals in $T < -20^\circ C$.

Ice nucleation processes through homogeneous and
heterogeneous nucleation and the supersaturation di-
agnosis with a time step that does not resolve vapor-
aerosol interaction can be considered the weakest links
of the model. The spatial distribution and concentra-
tion of IN and supersaturation determines the habit of
ice crystals and their concentration. Even if SHIPS is
proved to be useful to predict habit and its evolution in
multidimension Eulerian models, the inappropriate ice
nucleation process and supersaturation could lead the
simulation to a different realization of solid hydrometeors.

SHIPS is the first proposed scheme for multidimen-
sional CRMs to explicitly evolve the arbitrary ice crys-
tal habit. The simulations with SHIPS including aggre-
gation and riming processes will be validated and im-
proved over time with direct and indirect observations
of solid hydrometeors. This paradigm of microphysics
methodology, a continuous-property approach, offers
great potential to atmospheric modeling and data as-
simulation. In the future, the most likely source of high
resolution of microphysical observations will be from
our spaceborne remote sensing platforms. The usefulness
of their observations, particularly of clouds, lies in
our ability to physically model what they observe and
so the physical connection with traditional atmospheric
state variables. SHIPS is a step in the direction of being
able to explicitly model microphysical process and ul-
timately the attendant radiative effects that satellites
can observe. In the short term, SHIPS provides new
insights and understandings of the complex interactions
between ice crystal habit, aerosols, and cloud dynamics.

Currently, SHIPS is computationally more expensive
than bulk microphysics parameterization. As computa-
tional power continues to double every 1.5-2 yr, we
may be able to afford more integrity on cloud micro-
physics in CRMs.

Acknowledgments. The authors are very grateful to
Prof. J. P. Chen, Department of Atmospheric Sciences,
National Taiwan University, for his consultation on
coding hybrid-bin method. We are also thankful of the
comments and suggestions by the anonymous review-
ers. This research was supported by NASA (PMM-
0069-0153).

APPENDIX A

Mixing PPVs between Bins and Grid Cells

PPVs defined in section 2 have to be advected be-
tween mass bins in a physical and statistical manner
that preserves the history of a mean particle. This re-
quires that 1) the predicted variable is conserved under
mass- or concentration-weighted mixing, and 2) it pro-
duces a mean property of the bin that physically corre-
sponds to the hydrometeor having mass equal to the
mean mass of the bin. As the mass content components
and aerosol mass content components are proportional
the total mass content of hydrometeors, they auto-
matically satisfy the continuity equation for the total
mass content.

a. Length variable components

An important numerical challenge is how to transfer
the information on lengths of a particle between bins in
Eulerian microphysics scheme or between grid cells in the Eulerian dynamics framework. In both cases, a flux conservative numerical formulation represents the transfer as a conservative mixing between the bins in a grid cell or between the same mass bins of the surrounding grid cells. For mixing two groups of ice particles, one can write the conservation statement on the length variable component. Then, the mean length of a particle after the mixing must be retrieved. A requirement is that the length of a mean particle resulting from a mixture of particles contained in the two groups must correspond to the length for the mean mass of the mixture. Since the axis ratio and bulk crystal density of ice crystals are also constant within a bin from the implicit mass-sorting assumption, \( l_1^b \) must be proportional to \( \rho_1^b \), while the cubic of concentration weighted length is not. Therefore, \( l = \sqrt[l]{\frac{l_1^b}{N^b}} \) and \( m = \frac{\rho^b}{N^b} \) are consistent with the mass–length relationship defined by Eqs. (11)–(13). Furthermore, if the original and resulting particles have the same bulk crystal density and axis ratios, the conservation statement of \( l_1^b \) is equivalent to the mass continuity equation.

To show that \( l_1^b \) is better than \( l_1^c \) with regard to the requirement (2), the lengths of the representative hydrometeors were simulated with the two concentration-weighted variables by the hybrid-bin method. These were compared with the lengths of a single ice crystal simulated in a Lagrangian model. The vapor deposition process was simulated under water saturation at \(-15^\circ\text{C}\) and 700 hPa, employing five bins in the hybrid-bin method. According to Fig. A1a, the simulation with \( l_1^b \) tends to overestimate the maximum dimension, compared to the Lagrangian simulation. As the relative humidity increases, the prediction with \( l_1^c \) gives increasingly larger errors (not shown). On the other hand, Fig. A1b indicates that the simulation with \( l_1^b \) gives a solution closer to the Lagrangian model than one with \( l_1^c \).

To further validate the use of \( l_1^b \), the property of the bulk crystal density and the axis ratio of mixed particles is discussed using the example of mixing two groups of particles. By substituting mass–length relationships for each particle’s group into conservation equations, one can obtain:

\[
\bar{\rho}_3 = \left[ \frac{W_1(1 + \phi_2^a)^3 \rho_1 \phi_1^3 + W_2(1 + \phi_2^b)^3 \rho_2 \phi_2^3}{W_1(1 + \phi_2^a)^3 \rho_1 + W_2(1 + \phi_2^b)^3 \rho_2} \right]^{1/3},
\]

(A1)

\[
\bar{\rho}_3 = \frac{(1 + \phi_2^a)^{-3/2}}{W_1(1 + \phi_2^a)^{-3/2} \rho_1^{-1} + W_2(1 + \phi_2^b)^{-3/2} \rho_2^{-1}},
\]

(A2)

where \( W_1 = \varrho_1/\varrho_2 \), and \( W_2 = \varrho_2/\varrho_1 \). As Eq. (A1) indicates, \( \bar{\rho}_3 \) is bounded by the original axis ratio \( \phi_1 \) and \( \phi_2 \), and monotonically changes with \( W_1 \) and \( W_2 \) as well as \( \phi_1 \) and \( \phi_2 \). Also, simple calculations show that the quality of boundedness and monotonicity holds true for the bulk crystal density \( \bar{\rho}_3 \).

Examples of the axis ratio and bulk density after mixing the two bins containing planar crystals (group 1) and columnar crystals (group 2) are shown in Fig. A2. From Eq. (10), the following relationship between the bulk crystal density and axis ratios for the hexagonal crystal model can be derived:

\[
\rho_c = \frac{3\sqrt{3}\rho_1(1 - \phi)(1 + \phi)}{k_3(1 + \phi_2)^{3/2}}.
\]

(A3)
If \( \rho_i^h = \rho_i \) is assumed, the bulk crystal density \( \rho_c \) takes the maximum of 0.437 at \( \phi = 0.707 \) and \( \psi = 0 \). All particle groups in the cases 1–4 except for group 1 of case 3 satisfy the density–axis ratio relationship. For instance, case 1 shows that the case of mixing planar crystals of \( \phi_1 = 0.1, \rho_1 = 0.112, \phi_2 = 10.0, \rho_2 = 0.0112 \), and columnar crystals of \( \phi_2 = 10.0, \rho_2 = 0.0112 \) by about an equal amount of mass content gives a representative ice crystal with \( \rho_c = 0.437 \) and \( \phi_1 = 0.707 \) and \( \rho_c = 0.0169 \). Comparison of curves 2 and 5 or 4 and 6 of Fig. A2b indicates that the mixing gives a smaller bulk crystal density \( \rho_c \) than one obtained by substituting the resulting axis ratio \( \phi_3 \) into Eq. (A3). This suggests that the mixed particles can satisfy the mass–length relationship of the hexagonal crystal model only with smaller bulk density \( \rho_c \). The discrepancy in the bulk crystal density decreases as the difference of axis ratios between original particle groups decreases.

In conclusion, advection of \( \ell^{\phi}_{ij} \) is better than \( \ell^{\psi}_{ij} \) or other powered length because it is consistent with the mass–length relationship and implicit mass sorting assumption. The resulting average properties after mixing are bounded by properties of original particles and monotonically increase or decrease with mixed amounts.

b. Volume variable components

The conservation statement for the concentration-weighted volume \( V_{cs} \) is equivalent to that for mass conservation only if bins of the original and resulting particles have the same density \( \rho_c \). One can easily show that the bulk sphere density of the representative hydrometeor after mixing should be a bounded and monotonic function of the \( \rho_c \) of the original particle groups. The use of \( V_{cs} \) as the predicted PPV will result in an estimate of the mean property of the mixed particles in the Eulerian framework.

APPENDIX B

Description of Microphysical Process Models

The development of equations simulating the underlying liquid and ice microphysical processes follows Chen (1992) and CL1. It was modified to integrate the PPVs based on microphysical processes and suited to multidimensional CRMs. In the following, the current version of aerosol microphysics package [Aerosol Prediction System (APS)] and liquid-phase microphysics package [Spectral Liquid Prediction System (SLIPS)] of AMPS are described briefly, and then ice-phase microphysics package (SHIPS) is described.

a. Aerosol microphysics (APS)

Two types of aerosols are predicted: cloud condensation nuclei (CCN) and ice nuclei (IN). This research defines the partially soluble and insoluble aerosols as CCN, while pure insoluble aerosols are defined as IN. Therefore, for each grid cell there are two categories of internally mixed particles. In addition to the concentration and mass content, the soluble mass content is predicted as the PPV for each category. Currently the CCN and IN are predicted with the bulk approach due to the
computational cost associated with the bin approach. The accumulation mode of CCN is modeled with log-normal distribution with a fixed standard deviation, and the geometric mean size is diagnosed. IN is assumed to have one uniform size.

The sources and sinks considered are evaporation of hydrometeors and nucleation scavenging. If a hydrometeor evaporates and loses the water mass of the hydrometeor, the aerosol total and soluble mass contents are transferred back into the CCN or IN category, depending on the solubility. Once hydrometeors are nucleated, the total mass and soluble mass contents of CCN or IN are transferred into the bin of the nucleated hydrometeors. The deposition–condensation nucleation and contact-freezing nucleation are the sink for IN, while CCN is only deprived by cloud droplet activation. The fraction of activated cloud droplets is calculated with use of the dry critical radius formulated by Abdul-Razzak et al. (1998) based on the Kohler curve for mixed aerosols.

b. LIQUID-PHASE MICROPHYSICS (SLIPS)

The liquid-phase mass spectrum is divided into bins that are defined with mass boundaries. The prognostic variables are concentration and mass content, and aerosol mass content and soluble aerosol mass content are also predicted as PPVs. The hybrid-bin method is also applied to the liquid phase.

The processes simulated for the liquid spectrum is the vapor deposition process, the collision–coalescence process, and the collision–breakup process. The vapor deposition onto the activated droplets is calculated to compensate the time step. The CCN whose radius is between the critical radius and 99.5% of the lognormal size distribution is activated and condensed into multiple liquid bins. This enables the collision process among the liquid bins to start. The autoconversion process within a bin is not considered in this research. The collision processes are modeled by a quasi-stochastic approach, and coalescence–breakup processes are modeled based on Low and List (1982). There is no prediction of chemical reactions, which is different from CL1.

c. ICE-PHASE MICROPHYSICS (SHIPS)

1) ICE NUCLEATION

The ice nucleation process assigns the produced mass only to the ice crystal mass content component \( q_i \). Meyers et al.’s (1992) parameterization is used to estimate the number of pristine ice crystals due to deposition- and condensation-freezing nucleation. The concentration tendency (cm\(^{-3}\)) is given as

\[
\frac{\partial N}{\partial t} = \min\left(10^{-3} \exp\left(a_t + b_t 100 s_{\text{sat}}\right) N_{\text{IN}}\right),
\]

where \( a_t = -0.639, b_t = 0.1296, \) and \( s_{\text{sat}} \) is the supersaturation over ice. It is bounded by concentration of IN, \( N_{\text{IN}} \), predicted in the model. Similarly to Thompson et al. (2004), the conditions to turn on the nucleation are determined based on Schaller and Fukuta (1979): temperature is less than \(-5^\circ C\) and it is supersaturated over water, or it is more than 5% supersaturation over ice. The deposition- and condensation-freezing nucleation is a sink for IN. Initially, the radius and mass of the nucleated ice particle are set to those diagnosed from the uniform distribution of IN category predicted at the grid cell. This research calculates the growth of nucleated ice crystals by vapor deposition during the time step of nucleation with use of \( s_{\text{sat}} \), which is obtained from the saturation adjustment described in section 5. The length and mass growth of the nucleated crystals are calculated according to the local temperature and moisture as explained in section 4. The tendency of ice crystal mass content component is calculated by multiplying the mass change due to the IN and vapor deposition onto it by the concentration tendency. The tendencies of length and volume components are formed by multiplying the cubic lengths and volume by the concentration tendency. The tendencies of the nucleated mass content and concentration as well as PPVs are given to the mass bin that encompasses the resulting mean mass.

Contact nucleation is modeled using the model of Young (1974) that considers contacts by Brownian diffusion, thermophoresis, and diffusiophoresis following Cotton et al.’s (1986) treatment. Contact nucleation represents a sink to both the liquid hydrometeors and IN. The ice crystal created by contact nucleation process have mass corresponding to the freezing liquid hydrometeor, and conserve the axis ratio of semimajor and semiminor length of the freezing liquid hydrometeor, which is diagnosed by the empirical formula of Chuang and Beard (1990). The lengths are obtained from the mass–length relation of the hexagonal crystal \( m = 3\sqrt{3} \rho a^3 \). Therefore, contact nucleation can produce relatively large planar crystals from drizzles in warm temperature.

Immersion freezing is modeled based on Bigg’s (1953) stochastic hypothesis, following Reisin et al. (1996):

\[
N^b_i = N^b_i \left( 1 - \exp\left( -\frac{m^b_i}{\rho_w A} \exp[\bar{B}(T_0 - T)] \delta t \right) \right),
\]

(B2)
where \( N_{b}^{i} \) is the number of frozen drops of the \( b \)th bin in the mass spectrum of liquid hydrometeors, the parameters are \( A = 10^{-4} \text{cm}^{-3} \text{s}^{-1} \) and \( B = 0.66^{10^{-1}} \), and \( m_{b}^{i} \) is the mean mass of \( b \)th bin. The axis lengths and axis ratio of the nucleated ice crystal are calculated in the same way as contact nucleation. Then the concentration and mass content of frozen liquid hydrometeors as well as PPVs are transferred to the mass spectrum of solid hydrometeors using the subdistributions obtained with the two moments. Tendencies by immersion freezing are given by newly transferred prognostic variables divided by time step. The immersion freezing is a sink for liquid hydrometeors.

The secondary nucleation known as the Hallett-Mossop mechanism is not considered in this study since we do not consider riming process. Finally, the tendency by the ice nucleation process of SHIPS is given by adding tendencies of the three processes.

2) Melting–shedding process

For this paper the meltwater mass content component is not predicted. Heat tendency by melting is estimated based on the steady state of the heat budget:

\[
\left( \frac{\partial q}{\partial t} \right)_{\text{melting}} = \left( \frac{\partial q}{\partial t} \right)_{\text{diff,h}} + \left( \frac{\partial q}{\partial t} \right)_{\text{others}},
\]

where the term on the lhs is the heat tendency by melting, the first term on the rhs is the tendency by diffusion of heat through air, and the second term is the heat tendency by other processes. This paper only considers the heating rate due to vapor deposition for “other” processes, but it may include freezing by riming process and heat extracted for lowering temperature of rimed ice to temperature of parent ice surface. If the ambient temperature is above freezing \((T > T_{0})\), then it is reasonably assumed that the surface of a solid hydrometeor is coated by at least a thin layer of liquid water. Substituting

\[
\left( \frac{\partial q}{\partial t} \right)_{\text{diff,h}} = 4\pi C_{k \alpha} f_{0}(T - T_{s}),
\]

\[
\left( \frac{\partial q}{\partial t} \right)_{\text{diff,m}} = 4\pi C_{L \alpha} G(T, p) f_{w} s_{wv},
\]

into Eq. (B3) with surface temperature \( T_{s} = T_{0} \) gives the melting tendency for the representative hydrometeor in a bin:

\[
\frac{dm_{W}}{dt} = \left( \frac{dq}{dt} \right)_{\text{melting}}.
\]

If the mass component \( m_{W} \) is predicted, and it exists, then the same approach can be used to obtain the tendency.

In cases where it is the subfreezing condition \((T < T_{0})\) and melting water does not exist, the melting tendency can be estimated by assuming it is 0 first in Eq. (B3). Then, \( T_{s} \) can be calculated from the heat balance. If \( T_{s} > T_{0} \), the hydrometeor is melting and it is assumed that \( T_{s} = T_{w} \). Then, the melting tendency is obtained by the method discussed above. Otherwise, the tendency is zero.

The meltwater \( m_{W} \) on the ice crystal over the time step is obtained by Eq. (B6). Knowing the mass of dry core of an ice crystal \( m_{\text{core}} = m - m_{W} \), the \( a \)- and \( c \)-axis lengths of the core are calculated from Eqs. (11)–(13) with an assumption of the same bulk crystal density and axis ratios as before melting. The shedding condition, shedded mass \( m_{\text{shed}} \) and size distribution of shedded drops are treated the same as by Chen (1992) and CL1. The circumscribing sphere volume after melting and shedding is estimated as

\[
\psi_{s} = \max\{m_{W} - m_{\text{shed}}\}/p_{w} + m_{\text{core}}/p_{t}.
\]

If the shedding occurs, the tendency of the mass content can be given by multiplying \(-m_{\text{shed}}/\delta t\) by the concentration of ice particles. The concentration tendency is 0, unless all mass of the representative hydrometeor is melted.

APPENDIX C

List of Symbols

Symbol description

- \( a \) is the \( a \)-axis length of the hexagonal crystal.
- \( a_{ab} \) is the ratio of mass ratios of adjacent boundaries.
- \( a_{h} \) is the diameter of the hexagonal part of the crystal without dendritic arm lengths.
- \( A_{c}, A_{r} \) is the area defined by the ratio of projected area of a hydrometeor and that of circumscribing spheroid, respectively.
- \( c \) is the \( c \)-axis length of the hexagonal crystal.
- \( C, C(a, c) \) is the capacitance model of a spheroid with \( a \)- and \( c \)-axis lengths, respectively.
- \( d \) is the dendritic arm length of the hexagonal crystal.
- \( f_{w}, f_{r} \) is the mean ventilation coefficient for heat diffusion and vapor diffusion, respectively.
- \( f_{kn} \) is the mass transfer correction factor for the kinetic process.
- \( G(T, p) \) is the thermodynamic function.
slope of linear distribution within a mass bin

heat conductivity of air

arbitrary mass ratio of adjacent boundaries

coefficient associated with the sphere volume
eddy mixing coefficients for scalars characteristic length of the hydrometeor

order of the high-order filter

latent heat of evaporation of water

and melting of ice per unit mass, respectively
general symbol for concentration-weighted length and concentration-weighted cubic length for bth bin, respectively

concentration weighted cubic a-axis length, cubic c-axis length, and cubic dendritic arm length for the bth bin, respectively

number of particles per unit of volume and mass

concentration of particles (number of particles per unit volume of air) in bth mass bin

concentration of the particle group i

concentration of the bth bin in the liquid spectrum

number concentration of IN

Reynolds number

mass of a hydrometeor
total, soluble, and insoluble mass of aerosols within a solid hydrometeor, respectively

mass of dry core of an ice crystal after melting

mass of shedded water from an ice particle

mass component produced by the vapor deposition process onto an ice crystal

mass component produced by the riming process for a solid hydrometeor

mass component produced by the aggregation process for a solid hydrometeor

liquid mass component produced by melting on a solid hydrometeor

mean mass defined by $\rho^b N^b$

mean mass defined by $\rho^b N^b$ left and right mass boundaries of bth bin, respectively

atmospheric pressure

specific quantity of the ice parameter $n$ in mass bin $b$

area ratio $A_i / A_c$

supersaturation over water and ice, respectively

source term by microphysics processes temperature of ambient atmosphere surface temperature of a hydrometeor melting temperature of ice velocity components volume of the spheroid circumscribing a hydrometeor terminal velocity of the representative hydrometeor in the bth bin concentration-weighted circumscribing volume weights defined by mass content for group $i$

the Cartesian grid unit tensor

Davis number

aspect ratio defined as ratio of semimajor axis length to semimajor axis length of a spheroid circumscribing a hydrometeor inherent growth ratio time step for the microphysical processes dynamic viscosity high-order numerical mixing coefficient density of moist air bulk crystal density (mass of an ice crystal per volume of a sphere circumscribing the crystal)

density of ice and water, respectively bulk density of the hexagonal crystal model bulk sphere density (mass of particle per volume of a sphere circumscribing the particle)

total and soluble mass content (mass of particles per unit volume of air) of aerosols within solid hydrometeors in bth mass bin, respectively

mass content of the particle group i quantity per unit volume of air of the ice parameter $n$ in the mass bin $b$

mass content of the bth mass bin mass content components (integrated mass components over mass for a bin)
axis ratios of hexagonal ice crystal, $c/a$ and $d/a$, respectively; axis ratios are defined as the ratio of lengths along crystallographic axes of an ice crystal property of the representative hydrometeor at mean mass of the bin or group such as $\bar{a}$, $\bar{c}$, $\bar{p}_i$, $\bar{\psi}$

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