Parameterization of the Autoconversion Process. Part II: Generalization of Sundqvist-Type Parameterizations

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ABSTRACT

Existing Sundqvist-type parameterizations, which only consider dependence of the autoconversion rate on cloud liquid water content, are generalized to explicitly account for the droplet concentration and relative dispersion of the cloud droplet size distribution as well. The generalized Sundqvist-type parameterization includes the more commonly used Kessler-type parameterization as a special case, unifying the two different types of parameterizations for the autoconversion rate. The generalized Sundqvist-type parameterization is identical with the Kessler-type parameterization presented in Part I beyond the autoconversion threshold, but exhibits a more realistic, smooth transition in the vicinity of the autoconversion threshold (threshold behavior) in contrast to the discontinuously abrupt transition embodied in the Kessler-type parameterization. A new Sundqvist-type parameterization is further derived by applying the expression for the critical radius derived from the kinetic potential theory to the generalized Sundqvist-type parameterization. The new parameterization eliminates the need for defining the driving radius and for prescribing the critical radius associated with Kessler-type parameterizations. The two-part structure of the autoconversion process raises questions regarding model-based empirical parameterizations obtained by fitting simulation results from detailed collection models with a single function.

1. Introduction

Rain in liquid water clouds is initiated by the autoconversion process whereby larger droplets with higher settling velocities collect smaller droplets and become embryonic raindrops. Accurate parameterization of the autoconversion process in atmospheric models of various scales [from large-eddy simulations (LES) to global climate models] is important for understanding the interactions between cloud microphysics and cloud dynamics (e.g., Chen and Cotton 1987), for the forecasting of the freezing drizzle formation and aircraft icing (Rasmussen et al. 2002), and for improving the treatment of clouds in climate models (Rotstayn 2000). The effort to improve the parameterization of the autoconversion rate has been recently reinforced by an increasing in-

terest in cloud–climate interactions, and particularly in studies of the second indirect aerosol effect (Boucher et al. 1995; Lohmann and Feichter 1997; Rotstayn 2000; Rotstayn and Liu 2005).

Part I of this series (Liu and Daum 2004, hereafter Part I) was mainly focused on improving Kessler-type parameterizations because of their widespread use. The Kessler-type autoconversion parameterizations that had been widely used in cloud-related modeling studies were theoretically derived and analyzed by applying the generalized mean value theorem for integrals to the general collection equation. The approximations implicitly assumed in these parameterizations, their logical connections and the gradual improvements were revealed by the derivations. A new parameterization was analytically derived by eliminating the incorrect assumption of fixed collection efficiency inherent in the previous Kessler-type parameterizations. The new Kessler-type parameterization exhibits stronger dependence of the autoconversion rate on the cloud liquid water content and the cloud droplet number concentra-

tion, explicitly accounts for relative dispersion of the cloud droplet size distribution, and better represents the physics of the autoconversion process compared to previous Kessler-type parameterizations.

Despite all these improvements, the new Kessler-type parameterization still suffers from a deficiency shared by all the Kessler-type parameterizations: a discontinuous, unrealistic representation of the threshold behavior of the autoconversion process by a Heaviside step function. Sundqvist (1978) proposed an alternative type of autoconversion parameterization that exhibits a smooth threshold behavior. Sundqvist-type parameterizations, however, are much less developed in comparison with Kessler-type parameterizations. Cloud liquid water content is the only variable that is explicitly considered in Sundqvist-type parameterizations, limiting their applicability and precluding use in studies of the second indirect aerosol effect. In this contribution, existing Sundqvist-type parameterizations are generalized to explicitly account for the cloud droplet concentration, the liquid water content, and relative dispersion. It is shown not only that the generalized Sundqvist-type parameterization describes the threshold behavior more realistically, but also that a Kessler-type parameterization becomes a special case of the corresponding generalized Sundqvist-type parameterization. A new Sundqvist-type parameterization is then derived by combining some results from Part I and the analytical expression for the critical radius recently derived in Liu et al. (2004).

2. Threshold behavior and its representation

It has been known since the 1960s (e.g., Kessler 1969) that the autoconversion process exhibits a threshold behavior. The threshold behavior intuitively conceived by Kessler has been put on a solid theoretical foundation by the kinetic potential theory recently formulated for the initiation of warm rain (McGraw and Liu 2003, 2004). Accordingly, the autoconversion rate (P) can be generically expressed as

$$P = P_0 T, \qquad (1)$$

where $T \leq 1$ denotes the function that describes the threshold behavior (hereafter threshold function), and P_0 represents the rate of change of the liquid water content beyond the threshold (rate function hereafter). For Kessler-type parameterizations,

$$T_K = H(r_m - r_c), \qquad (2)$$

where H is the Heaviside step function introduced to force the autoconversion rate to be zero when the driving radius r_m is less than the critical radius r_c. There are differences among various Kessler-type parameteriza-

tions as to the autoconversion function P_0 and the definition of the driving radius r_m (see Part I for a detailed discussion). Note that r_m and r_c become the liquid water content and critical liquid water content respectively for the original Kessler parameterization that considers only the dependence of autoconversion rate on the liquid water content (Kessler 1969).

However, the all-or-nothing representation of the threshold behavior by the Heaviside step function used in Kessler-type parameterizations, including that presented in Part I, does not accurately describe the threshold behavior; the change of the autoconversion rate near the threshold is expected to be smooth, not discontinuous as characterized by the Heaviside step function (Wood and Blossey 2005; Liu and Daum 2005). Sundqvist (1978) proposed an alternative expression for the autoconversion rate

$$P_S = c_s L T_S, \qquad (3a)$$

$$T_S = 1 - \exp\left[-\left(\frac{L}{L_c}\right)^2\right], \qquad (3b)$$

where L is the cloud liquid water content, c_s is an empirical constant in s^{-1}, and L_c is the threshold cloud liquid water content. A slightly different threshold function was proposed by Del Genio et al. (1996)

$$T_S = 1 - \exp\left[-\left(\frac{L}{L_c}\right)^4\right]. \qquad (4)$$

It is worth stressing that the primary distinction between the Sundqvist parameterization and the original Kessler parameterization lies in the treatment of the threshold function. The Sundqvist threshold function as described by (3b) is smoother than the Heaviside $H(L - L_0)$ associated with the original Kessler parameterization, and seems more appropriate for describing the threshold behavior of the autoconversion process.

3. Generalized Sundqvist-type threshold function

It is straightforward to generalize the above Sundqvist-type parameterizations. First, a general threshold function that includes the above two Sundqvist-type threshold functions as special cases is defined as

$$T_S = 1 - \exp\left[-\left(\frac{L}{L_c}\right)^\mu\right], \qquad (5)$$

where $\mu \geq 0$ is introduced as an empirical constant. As will become clear, this simple generalization is useful for understanding the relationship of Kessler-type parameterizations to Sundqvist-type parameterizations.

Second, unlike the original Kessler parameterization that has been extended to include the cloud droplet concentration and relative dispersion as independent

variables, Sundqvist-type parameterizations remain limited to the liquid water content only, and can be extended to explicitly account for the droplet concentration and relative dispersion using an approach that is similar to that used for the extension of the original Kessler parameterization. Briefly, if the critical liquid water content is defined as

$$L_c = Nm_c = N\frac{4\pi\rho_w}{3}r_c^3, \qquad (6)$$

where N is the cloud droplet number concentration, m_c is the critical mass, and ρ_w is the water density, then, (5) can be rewritten as

$$T_S = 1 - \exp(-x_S^\mu), \qquad (7a)$$

$$x_S = \frac{\overline{m}}{m_c} = \left(\frac{r_3}{r_c}\right)^3, \qquad (7b)$$

where $\overline{m} = L/N$ is the mean mass per droplet, r_3 is the mean volume radius, and x_S is the dimensionless mass ratio. The role of the dimensionless mass ratio for Sundqvist-type parameterizations is similar to that of "$r_m - r_c$" for Kessler-type parameterizations. Evidently, (5) is a special case of (7) when the cloud droplet concentration is fixed.

Figure 1 shows the threshold function T_S as a function of the dimensionless mass ratio for different values of μ. Also shown for comparison are the ratios of the autoconversion rates calculated from measurements of cloud droplet size distributions to the corresponding values of the Liu–Daum rate function. The observationally estimated autoconversion rates are calculated by explicit solution of the stochastic collection equation from droplet size distributions measured in stratiform boundary layer clouds Wood (2005). It is obvious from Fig. 1 that T_S approaches the Heaviside step function when μ increases, suggesting that the more commonly used Kessler-type parameterizations can be considered as an approximate limit of the corresponding Sundqvist-type parameterization. Furthermore, it can be argued that the smooth threshold function T_s describes the threshold behavior more accurately than the discontinuous Heaviside function assumed for Kessler-type parameterizations. The scatter of the data points is likely due to differences in values of relative dispersion, but may also be indicative of differences in the definitions of the autoconversion rate integral used in the Wood (2005) and Liu and Daum (2004) studies (Wood and Blossey 2005). Further discussion of this is presented in section 5.

Coupling of (7) to any rate function will yield a generalized Sundquist-type parameterization that encompasses the traditional Kessler- and Sundqvist-type parameterizations. For example, the combination of (7)
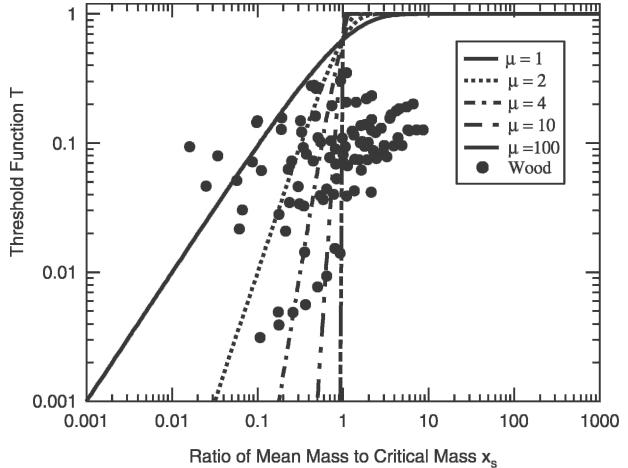

FIG. 1. Illustration of the Sundqvist-type threshold function. The dots denote the ratios of the autoconversion rates calculated by applying measured cloud droplet size distributions to the collection equation (Wood 2005) to the corresponding Liu–Daum rate functions calculated using the measured liquid water contents, droplet concentrations, and relative dispersions.

with the Liu–Daum rate function P_0 derived in Part I leads to a generalized Sundqvist-type parameterization given by

$$P_S = \kappa\beta_6^6 N^{-1}L^3[1 - \exp(-x_S^\mu)], \qquad (8a)$$

$$\beta_6 = \left[\frac{(1 + 3\varepsilon^2)(1 + 4\varepsilon^2)(1 + 5\varepsilon^2)}{(1 + \varepsilon^2)(1 + 2\varepsilon^2)}\right]^{1/6}, \qquad (8b)$$

where $\kappa = 1.1 \times 10^{10}$ g^{-2} cm^3 s^{-1} is a constant in the Long collection kernel (Long 1974), and ε is the relative dispersion of the cloud droplet size distribution (L and N are also in cgs units).

According to the preceding analysis, the generalized Sundqvist-type parameterization includes the Liu–Daum Kessler-type parameterization presented in Part I as a limiting case of μ approaching $\propto$. To illustrate this point, Fig. 2 shows the autoconversion rate as a function of the cloud liquid water content calculated from (8) for different values of μ. The critical radius r_c has been considered an empirical constant in modeling studies using Kessler-type parameterizations; a value of $r_c = 10$ μm is used in the calculations. The solid ($N = 50$ cm^{-3}) and dashed ($N = 500$ cm^{-3}) lines are shown to exemplify marine and continental clouds, respectively. It is evident from Fig. 2 that the generalized Sundqvist-type parameterization gradually approaches the form of the corresponding Kessler-type parameterization when the exponent μ increases, unifying the two traditionally different types of autoconversion parameterizations. It is also evident that the threshold liquid water content increases with increasing cloud droplet con-
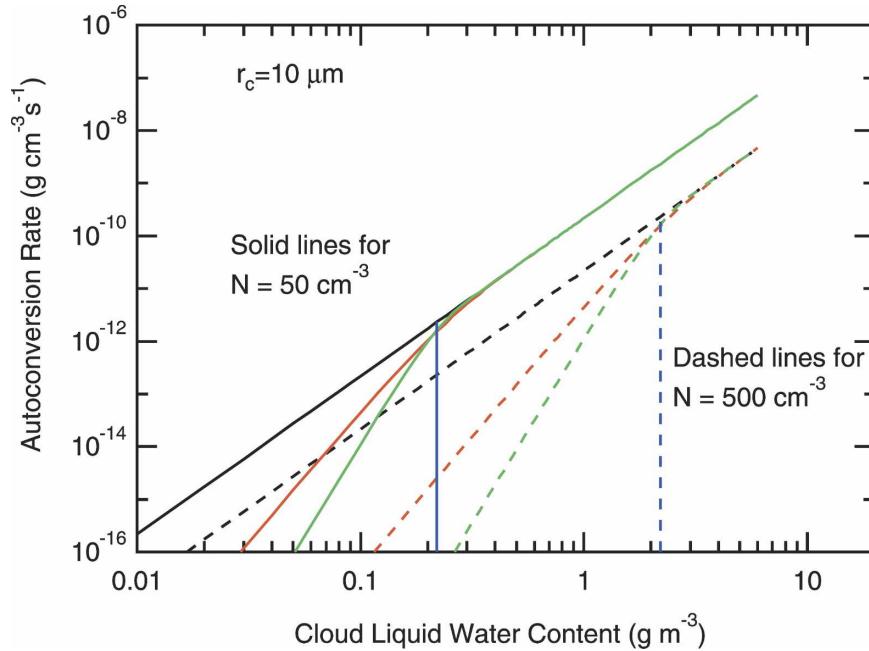
FIG. 2. Illustration of the generalized Sundqvist-type parameterization. The solid and dashed lines represent cases with the cloud droplet concentration $N = 50$ cm^{-3} and $N = 500$ cm^{-3}, respectively. The black, red, green, and blue lines represent the Liu–Daum rate function P_0, $\mu = 2$, 4, and the limit of $m \to \infty$, respectively. The threshold liquid water content L_c increases linearly with the cloud droplet concentration: $L_c = (4/3)\pi\rho_w r_c^3 N$.

centrations, instead of being a constant as assumed in the original Sundqvist parameterization. This is qualitatively consistent with the assumption used in Del Genio et al. (1996) that marine clouds have a smaller threshold liquid water content compared to their continental counterparts.

4. Expression for critical radius and new parameterization

The critical radius r_c has been considered an empirical constant and arbitrarily tuned in modeling studies using Kessler-type parameterizations. To remove this deficiency, Liu et al. (2004) recently derived an analytical expression that relates r_c to cloud liquid water content and droplet concentration,

$$r_c = \left(\frac{3}{4\pi}\right)^{1/3} \frac{\nu^{1/3}\beta_{con}^{1/6}}{\kappa^{1/6}} N^{1/6}L^{-1/3}, \qquad (9)$$

where $\nu = 3.0 \times 10^{-23}$ (g) is the mass of an individual water molecule, and $\beta_{con} = 1.15 \times 10^{23}$ (s^{-1}) is the average condensation rate constant. The derivation is based on the kinetic potential theory, in which r_c corresponds to the kinetic potential barrier (McGraw and Liu 2003, 2004). See also McGraw and Liu (2004) for an alternative derivation of (9). Application of (9) yields

expressions for the critical mass and the dimensionless mass ratio, respectively,

$$m_c = \left(\frac{4\pi\rho_w}{3}\right)r_c^3 = \frac{\rho_w\nu}{\kappa^{1/2}}\beta_{con}^{1/2}N^{1/2}L^{-1}, \qquad (10)$$

$$x_S = \frac{\kappa^{1/2}}{\rho_w\nu\beta_{con}^{1/2}} N^{-3/2}L^2 = 1.03 \times 10^{16}N^{-3/2}L^2. \qquad (11)$$

Substitution of (11) into (7) and (8) yields the generalized Sundqvist-type threshold function

$$T_S = \{1 - \exp[-(1.03 \times 10^{16}N^{-3/2}L^2)^\mu]\}. \qquad (12)$$

A combination of (12) with the Liu–Daum rate function yields a new generalized Sundqvist-type parameterization given by

$$P_S = \kappa\beta_6^6 N^{-1}L^3\{1 - \exp[-(1.03 \times 10^{16}N^{-3/2}L^2)^\mu]\}. \qquad (13)$$

It is noteworthy that except for μ there is no tunable parameter in this new parameterization, in contrast to the Kessler-type parameterization that needs to define the driving radius. Furthermore, the new Sundqvist-type parameterization actually encompasses the new Kessler-type parameterization in the limit when $\mu \to \infty$.

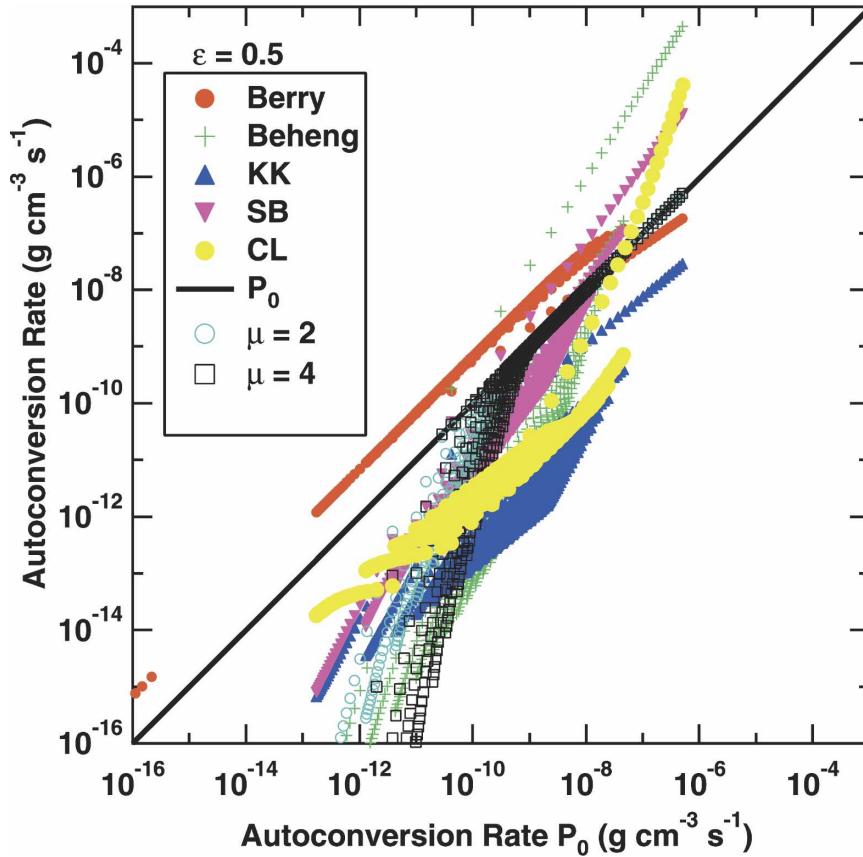It was argued in Part I that the driving radius in the

FIG. 3. Illustration of the new Sundqvist-type parameterization along with the previous parameterizations compared in Fig. 2 of Part I. The two typical examples of the new Sundqvist-type parameterization shown here correspond to $\mu = 2$, and 4, respectively. Berry = Berry (1968); Beheng = Beheng (1994); KK = Khairoutdinov and Kogan (2000); SB = Seifert and Beheng (2001); CL = Chen and Liu (2004); P_0 = Liu–Daum rate function. The Heaviside threshold function for the Kessler-type parameterizations, which will result in a steep, discontinuous fall of the autoconversion rate at the threshold, is not shown in this figure.

Kessler-type autoconversion parameterization is the mean radius of the sixth-moment r_6, instead of the mean volume radius r_3 as assumed in previous Kessler-type parameterizations. For the Liu–Daum Kessler-type parameterization (r_6 scheme), the threshold liquid water content is given (Rotstayn and Liu 2005),

$$L_c = \frac{4}{3} \pi \rho_w \beta_6^{-3} r_c^3 N. \tag{14}$$

Because β_6 is larger than one for typical clouds, the Liu–Daum Kessler-type parameterization leads to a threshold liquid water content smaller than that corresponding to the r_3 scheme. Figure 2 suggests that the r_6 scheme with a smaller L_c seems to approximate the threshold behavior described by the typical Sundqvist-type parameterizations ($\mu = 2$ and 4) better than the corresponding r_3 scheme. This result suggests that according to their representation of threshold behavior, the r_6 scheme is preferred to the r_3 scheme when using

Kessler-type parameterizations, although neither is as accurate as the corresponding generalized Sundqvist-type parameterization.

5. Comparison

To further examine the new Sundqvist-type parameterization, the results presented in Fig. 2 of Part I are updated by adding the autoconversion rates derived from (13) with the two typical values of $\mu = 2$, 4. The updated results are shown here in Fig. 3. Also added in Fig. 3 is the most recent Chen–Liu autoconversion parameterization derived from fitting detailed microphysical simulations (Chen and Liu 2004). It is evident from Fig. 3 that the differences between the Liu–Daum rate function, the Kessler-type parameterization, and the new Sundqvist parameterizations disappear beyond the threshold as expected. The primary difference between the Kessler-type and the new Sundqvist-type pa-

rameterizations lies in their description of the threshold behavior. The new Sundqvist-type parameterization with the two commonly used values of $\mu = 2$ and 4 seems to describe the threshold behavior more realistically than the Heaviside step function associated with the corresponding Kessler-type parameterization, which is the limit of the Sundqvist-type parameterization when the parameter μ approaches $\propto$.

In view of the difficulty of validating autoconversion parameterizations using data from ambient clouds, model-based empirical parameterizations have been considered among the most accurate parameterizations despite the various deficiencies associated with such schemes as discussed in Part I. This common wisdom seems reasonable at first glance because detailed models solve the collection equation exactly and use the most accurate collection kernel available. The results discussed above, however, raise critical questions regarding this traditional belief. A single function such as a power law has often been used in the regression procedure to obtain empirical parameterizations (e.g., Berry 1968; Beheng 1994; Khairoutdinov and Kogan 2000). However, the autoconversion rate actually consists of two distinct parts (P_0 and T) that are described by very different functions. Therefore, any fit with a single function such as the commonly used power law will somewhat distort the parameterized autoconversion rate obtained this way.

It is noteworthy that although the concept of the autoconversion process has been well known qualitatively, there is no generally accepted quantitative definition. The striking differences among various parameterizations shown in Fig. 3 may be closely related to different definitions used in deriving autoconversion parameterizations. In general, there are three different approaches that have been used to mathematically define the autoconversion rate. First, according to Kessler's original ideas, autoconversion starts once some threshold is crossed, and the autoconversion rate represents the growth rate by the collection process integrated over drops from the critical radius to sizes that are large enough to fall as small raindrops. This study, along with Part I and Liu et al. (2005), demonstrates that various phenomenological Kessler- and Sundqvist-type parameterizations can be theoretical derived from this definition under certain assumptions on the collection kernel. This definition is favorable considering its easy analytical treatment and clear partition of the autoconversion rate into threshold function and rate function. Berry (1968) introduced the second definition that expresses the autoconversion rate as the ratio of the cloud liquid water content to the characteristic time that the predominant radius of the cloud

droplet system reaches some value (e.g., 50 or 100 μm). The third definition was proposed by Beheng and further separates self-collection of cloud droplets (collected cloud droplets remain as cloud droplets) from the autoconversion process, (e.g., Beheng 1994). This third definition has been mainly used in obtaining simulation-based parameterizations because of its difficulty for analytical analysis. Simulation-based parameterizations obtained using this definition, however, are highly sensitive to the separation radius r_0 that is introduced to distinguish cloud droplets from raindrops, and there appears to be no general agreement as to the value of the separation radius. Values from 20 μm (e.g., Wood 2005) to 25 μm (Khairoutdinov and Kogan 2000) to 50 μm (e.g., Beheng 1994; Chen and Liu 2004) have been used in different studies. Part of the large discrepancies among those simulation-based parameterizations using the Beheng definition of the autoconversion rate shown in Fig. 3 may be indicative of the differences in the separation radius assumed in simulations. It is also puzzling to note that there are even significant differences between the Beheng and the Chen–Liu parameterizations, which uses the same separation radius. More research is evidently needed to resolve this important issue of quantitative definition of the autoconversion process, which should be in the context of easy use for atmospheric models, and consistent with the other processes (e.g., accretion) that need to be parameterized in atmospheric models as well.

6. Concluding remarks

It is briefly argued that the autoconversion rate P can be generally expressed as a product of two distinct parts: the rate P_0 and the threshold function T, and that existing phenomenological parameterizations can be classified into either Kessler- or Sundqvist-type according to their threshold functions. Existing Sundqvist-type parameterizations are first generalized by introducing an empirical exponent μ, and then extended to explicitly account for the effects of the cloud droplet concentration and relative dispersion on the autoconversion rate. The generalized Sundqvist-type parameterization includes the corresponding Kessler-type parameterization as a limiting case of $\mu \to \propto$, unifying the two traditionally different ways of parameterizing the autoconversion rate.

A new Sundqvist-type parameterization is further derived by combining the autoconversion function derived in Part I, the expression for the critical radius derived in Liu et al. (2004), and the generalized Sundqvist-type threshold function. The new parameterization improves the representation of the threshold func-

tion, explicitly considers both liquid water content and droplet concentration, and removes the need for defining the driving radius and prescribing the critical radius associated with Kessler-type parameterizations. Further examination of the two-part structure of the autoconversion process reveals that those empirical parameterizations obtained by fitting simulation results from detailed collection models with a single function such as a power law likely distort the representation of either the autoconversion function or the threshold function. The improvements of the autoconversion function P_0 derived in Part I, the improved representation of the threshold behavior, and the possible distortion of the model-based empirical parameterizations lend collective support to the new Sundqvist-type parameterization.

The treatment of the threshold behavior essentially determines whether or not warm clouds precipitate in atmospheric models, and therefore is critical for evaluating the second indirect aerosol effect. This has been demonstrated by a recent global climate modeling study, which shows a 27% reduction of the second indirect aerosol effect when the previous Kessler-type threshold function is replaced with a new Kessler-type threshold function (Rotstayn and Liu 2005). The new Sundqvist-type parameterization encompasses all existing types of autoconversion parameterizations when the exponent μ varies from 0 to $\propto$; this feature of the new Sundqvist-type parameterization can be utilized to further such studies by varying the exponent μ.

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