

A Comparison of the Conservation of Number Concentration for the Continuous Collection and Vapor Diffusion Growth Equations Using One- and Two-Moment Schemes

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ABSTRACT

One- and two-moment parameterizations are integrated over hydrometeor diameters $D(0, \infty)$ for vapor diffusion and the continuous collection growth processes. For the conditions specified, the total number concentration of collector particles should be conserved. To address the problem, the gamma distribution function is used for the spectral density function. Predicted variables can include total mixing ratio q , total number concentration N_t , and characteristic diameter D_n (inverse of the distribution slope λ). In all of the cases, the slope intercept n_o is diagnosed or specified. The popular one- and two-moment methods that are explored include the one-moment method in which q is predicted, n_o is specified, and N_t and D_n are diagnosed; the one-moment method in which q is predicted, D_n is specified, and N_t and n_o are diagnosed; the two-moment method in which q and D_n are predicted and N_t and n_o are diagnosed; and the two-moment method in which q and N_t are predicted and n_o and D_n are diagnosed. It is demonstrated for the processes examined that all of the schemes 1) fail to conserve N_t for the collector particles when N_t should be conserved and 2) have other unphysical attributes, except for the two-moment method in which q and N_t are predicted. In recent years there has been a dramatic increase in the use of more-sophisticated microphysical parameterizations in cloud, mesoscale, and climate models, and it is increasingly important for a model user to be cognizant of the strengths and weaknesses of the parameterizations in complex models.

1. Introduction

Four parameterization techniques are selected to demonstrate their behavior when used for vapor diffusion growth and the continuous collection growth equations. With the continuous collection growth equation, it is assumed that the available number of droplets that can be collected is infinite, that all droplets collected are the same size, and that all droplets are collected at the same rate for all like collector drops, the latter of

which do not experience self-collection. The vapor diffusion growth equation describes depositional growth of a spectrum of ice particles without nucleation of new ice particles. With these equation specifications, the total number concentration for the collector drops or ice particles ideally should be conserved for any parameterization technique used. It is shown, however, that total number concentration is only conserved for one parameterization technique and the rest fail. The specific techniques evaluated are described below.

In the past few years, there has been a rapid increase in the use of more-complex one-moment schemes, as well as new two-moment schemes, in microphysics parameterizations. Therefore, we feel compelled to compare objectively the one-moment and two-moment

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methods that are being widely used by the research and operational community, including those developed or used by, for example, Srivastava (1967, 1971), Passarelli (1978), Passarelli and Srivastava (1979), Lin et al. (1983, hereinafter LFO), Rutledge and Hobbs (1983, hereinafter RH), Ferrier (1994), Mitchell (1988, 1994), Walko et al. (1995), Meyers et al. (1997), Reisner et al. (1998), Cohard and Pinty (2000), van den Heever (2002), van den Heever and Cotton (2004), Gilmore et al. (2004a,b), and many more.

To examine the problem stated above, the gamma distribution function is used for the hydrometeor spectral density function. The main properties of the size distribution may be described by variables that represent the hydrometeor distribution characteristics, including the total mixing ratio q , total number concentration N_t , characteristic diameter D_n (the inverse of the distribution slope λ), and the slope intercept n_o (Walko et al. 1995). Table 1 shows what is predicted, specified as constant, and/or diagnosed in the commonly used schemes, as well as other schemes that could be used.

In this paper, the following four commonly used parameterization schemes (Table 1) are evaluated:

- 1) a one-moment method in which q is predicted, n_o is specified as a constant, and N_t and D_n are diagnosed (scheme A);
- 2) a one-moment method in which q is predicted, D_n is specified as a constant, and N_t and n_o are diagnosed (scheme B);
- 3) a two-moment method in which q and D_n are predicted and N_t and n_o are diagnosed (scheme E); and
- 4) a two-moment method in which q and N_t are predicted and n_o and D_n are diagnosed (scheme F).

The similarities and differences of these schemes are evaluated by idealized integration of the LFO form of

each of the continuous collection growth and vapor diffusion growth equations.

A control scheme is needed to make comparisons, and, because we do not know what scheme is best for it, we need to do some analysis concerning solution behaviors. If we make the assumption of either a variable or steady production rate of q by continuous collection or vapor diffusion growth, then scheme F will conserve N_t by definition. Because we know scheme F has this property, we select it as the reference or control scheme. Relative differences (RDs) between each of the schemes and scheme F are computed for dq/dt , q , D_n , N_p , and n_o , where t is time.

In section 2, for completeness, mathematical definitions are provided for the variables described above. In section 3, integration results and scheme comparisons are provided and discussed. In section 4, the conclusions are presented.

2. Mathematical definitions

In the following, several familiar moments are defined. Note that in this paper D_n is defined in terms of unit length, whereas in LFO, RH, Passarelli (1978), Passarelli and Srivastava (1979), and Mitchell (1988), and other references, $\lambda = 1/D_n$ is defined in terms of “per unit length.” This difference has a pronounced influence on the way the equation for dD_n/dt appears in their works and our paper. It will appear as if there is a sign error for dD_n/dt when compared with Passarelli (1978), Passarelli and Srivastava (1979), and Mitchell (1988), but this is not the case. In several of the gamma functions $\Gamma(x)$, there is the appearance of a missing “1” that should be added to x ; it has to do with the way the gamma distribution function is written relative to other papers (e.g., Passarelli 1978; Passarelli and Srivastava 1979; Mitchell 1988).

TABLE 1. Variables predicted and specified as constant in microphysical parameterizations; here C = constant, P = predicted, and blank spaces are floating variables that are or can be diagnosed.

Scheme	No. of predicted moments	Water content	Intercept	Slope	No. concentration	Reference
A	1	P	C			LFO, RH, Walko et al. (1995), Gilmore et al. (2004a,b)
B	1	P		C		van den Heever and Cotton (2004), Stalker and Knupp (2003)
C	1	P			C	Not used to our knowledge
D	2	P	P			Not used to our knowledge
E	2	P		P		Passarelli (1978), Srivastava (1978), Passarelli and Srivastava (1979), Mitchell (1988)
F	2	P			P	Meyers et al. (1997), Ferrier (1994), Reisner et al. (1998), Ziegler (1985), Verlinde and Cotton (1993), Koenig and Murray (1976)

Four moments with respect to length over the diameter interval $D(0, \infty)$ are defined along with some other variables. The spectral density function is given by the gamma distribution. This function has been used by Walko et al. (1995), Meyers et al. (1997), and Cohard and Pinty (2000), among many others, and is given by

$$n(D) = \frac{N_t}{\Gamma(\nu)} \frac{1}{D_n} \left(\frac{D}{D_n} \right)^{\nu-1} \exp\left(-\frac{D}{D_n}\right), \quad (1)$$

where D is diameter (m), D_n has units of meters, N_t has units of inverse meters cubed, ν is a dimensionless distribution shape parameter, and Γ is the gamma function. The zeroth moment N_t , or number concentration, is defined over the interval for $D(0, \infty)$ by

$$N_t = \int_0^\infty n(D) dD. \quad (2)$$

The first moment or mean diameter is given by

$$D_{\text{mean}} = \frac{\int_0^\infty Dn(D) dD}{\int_0^\infty n(D) dD} = \frac{\Gamma(\nu+1)D_n}{\Gamma(\nu)} = \nu D_n, \quad (3)$$

where $\Gamma(\nu+1) = \nu\Gamma(\nu)$. The third moment, or mixing ratio q (kg kg^{-1}), can be defined over the interval $D(0, \infty)$ by

$$q = \frac{1}{\rho_o} \int_0^\infty m(D)n(D) dD = \frac{\alpha N_t \Gamma(\beta + \nu)}{\rho_o \Gamma(\nu)} D_n^\beta. \quad (4)$$

In all of the equations, for spheres, the mass is given by $m(D) = \alpha D^\beta$, where $\alpha = \rho\pi/6$ and $\beta = 3$. In the above, ρ and ρ_o are the densities of the particle and air, respectively. The variable D_n can be found in terms of N_t and q and other constants by using

$$D_n = \left[\frac{q\rho_o\Gamma(\nu)}{\alpha N_t\Gamma(\beta + \nu)} \right]^{(1/\beta)}. \quad (5)$$

Rearranging (4), the total concentration can be found in terms of q and D_n as

$$N_t = \frac{q\rho_o\Gamma(\nu)}{\alpha D_n^\beta\Gamma(\beta + \nu)}. \quad (6)$$

The slope intercept n_o ($\text{m}^{-\beta-\nu}$) can be found in terms of q and D_n as

$$n_o = \frac{q\rho_o\Gamma(\nu)}{\alpha\Gamma(\beta + \nu)D_n^{\beta+\nu}}. \quad (7)$$

Next, the sixth moment, or the reflectivity factor Z (for Rayleigh scatterers), for spheres can be prescribed over the interval $D(0, \infty)$ by

$$Z = \int_0^\infty D^{2\beta}n(D) dD = \frac{N_t\Gamma(2\beta + \nu)}{\Gamma(\nu)} D_n^{2\beta}. \quad (8)$$

Considerations for the dielectric should be used with ice particles. The general moment equation can be written for the interval $D(0, \infty)$ as described in Walko et al. (1995), for example. Although all of these moments are easy to derive and can be found elsewhere in the literature, they are presented here for completeness. Moreover, they are used to understand how the continuous collection and vapor diffusion equations behave.

Previous investigators (Passarelli 1978; Passarelli and Srivastava 1979; Mitchell 1988) have related the time rate of change of q and Z to arrive at an expression that can be used to derive an equation for $\partial D_n/\partial t$ for the vapor diffusion equation. We also use it with no complications for a simple continuous collection growth equation for spheres or disks. The derivation follows from basic steps for a sphere (Mitchell 1988, 1994). The main change between diffusion and collection is the value of δ , which is defined below for each of the processes considered. After some algebra, an equation for dD_n/dt is given by

$$\frac{dD_n}{dt} = \frac{D_n}{\beta q} \left[\frac{2\Gamma(\beta + \nu + \delta)\Gamma(\beta + \nu)}{\Gamma(\nu + \delta)\Gamma(2\beta + \nu)} - 1 \right] \frac{dq}{dt}. \quad (9)$$

3. Integration of microphysical growth equations and comparison of parameterization methods

a. Vapor diffusional growth of small ice spheres

We integrate the vapor diffusional growth equation for a spherical ice particle [symbols and values can be found in LFO, RH, and Pruppacher and Klett (1981, 1997)] for the interval over $D(0, \infty)$ using the following equation:

$$\frac{dq}{dt} = \int_0^\infty \frac{1}{\rho_o} \frac{2\pi D N_t f(S_x - 1)}{\left(\frac{L_s^2}{KR_v T^2} + \frac{1}{\rho_o q_{is} \Phi_v} \right)} n(D) dD. \quad (10)$$

Integration gives

$$\frac{dq}{dt} = \frac{1}{\rho_o} \frac{2\pi D_n N_t f(S_x - 1)}{\left(\frac{L_s^2}{KR_v T^2} + \frac{1}{\rho_o q_{is} \Phi_v} \right)}. \quad (11)$$

In (10) and (11), S_x is sublimation to liquid or ice, K is thermal conductivity, R_v is the gas constant for water vapor, q_{is} is the saturation mixing ratio over plane ice, and Φ_v is the diffusivity of water vapor. Also, f is the ventilation coefficient and is assumed to be unity for small particles. [This was done by Passarelli (1978), Passarelli and Srivastava (1979), and Mitchell (1988) so that (9) could be derived.]

Shapes other than spheres are not considered here but could be [e.g., a disk representing a plate crystal results in only a simple change to (10) and (11) (Pruppacher and Klett 1997)]. The time rate of change of N_t for vapor diffusion growth of a small ice sphere (mass increase), with no nucleation, is simply

$$\frac{dN_t}{dt} = 0. \tag{12}$$

Schemes A, B, E, and F (Table 1) are examined numerically by integrating (11) forward in time for 1200 s, using a 1-s time step for an ice sphere undergoing vapor deposition. The time step is kept small so that time truncation error is minimized. We specifically assume for this problem that $q_i = 1.0 \times 10^{-3} \text{ kg kg}^{-1}$ for cloud ice at time $t = 0$, $N_t = 1.0 \times 10^7 \text{ m}^{-3}$ at time $t = 0$, $f = 1$ (Passarelli 1978; Passarelli and Srivastava 1979; Mitchell 1988) and $\delta = 1$, $S_i = 1.05$ for all times, $\nu = 3$ for the distribution shape parameter, and $\rho_o = 1 \text{ kg m}^{-3}$ is density of air.

Sample values at $t = 300 \text{ s}$ of q , D_n , N_t , and n_o from schemes A, B, E, and F for diffusional growth of the ice spheres are shown in Table 2. The RDs against scheme F also are shown. The RDs range from around $O(10)\%$ to $O(1000)\%$!

Scheme F is examined to determine if it produces consistent solution trends and provides a reasonable comparison solution. With scheme F we find that $dq/dt > 0$ as prescribed and that $dN_t/dt = 0$ as it physically should be. Also, with scheme F, we find with (5) that D_n increases with time (which indicates larger characteristic as well as mean diameter with time), which is realistic, and with (7) that n_o decreases with time (given the above, this indicates that there are fewer small particles and more large particles with time, but that the total number concentration is constant), which also is cor-

rect. With regard to N_t and n_o , examination of all of the other schemes (Table 2) shows values and/or trends in RDs relative to scheme F. Schemes A, B, and E produce a larger number of particles than does scheme F, which implies the existence of more small particles (note the increase in n_o). In accordance with the increase in N_t and n_o , characteristic diameters D_n , and thus mean diameters for schemes A, B, and E, are all smaller at $t = 300 \text{ s}$ than for scheme F. This implies smaller characteristic diameter as well as mean diameters. Even though scheme A has an increasing D_n , and by definition scheme B has a constant D_n with time, neither is large enough in comparison with scheme F. These trends for schemes A, B, and E violate what should occur physically. From the results it is apparent that scheme A performs closest to the reference solution and scheme E has the greatest RDs.

b. Continuous collection growth of spherical graupel

The next process considered is continuous collection growth of spherical graupel (Wisner et al. 1972; Pruppacher and Klett 1981; LFO; RH; among others). There are numerous storm-scale prediction models [$O(1 \text{ km})$ or less for horizontal grid spacing] that include parameterizations that predict graupel, because the growth of graupel can have a large impact on total rainfall (e.g., Gilmore et al. 2004b). The growth of graupel occurs largely through collection or riming of cloud water (Gilmore et al. 2004b); thus, this is an important microphysical process to analyze. Some may argue that the form of this growth process presented here is very simple; however, many models still use it (certainly some models have more sophisticated parameterizations). Given its simplicity, there is some beauty in using this equation because the approximation $d[m(D)]/$

TABLE 2. Results from vapor diffusion growth of an ice sphere from 0 to 300 s. In columns A–F, the top values are the 300-s values and the bottom values are the errors relative to scheme F. RDs (in percent) are based on $100 \times |(\text{true} - \text{predicted}) \times \text{true}^{-1}|$, where true values are from scheme F and predicted values are from the other schemes.

Scheme	Initial values for all schemes	Final values and errors relative to scheme F			
		A: one moment, predict q , constant n_o	B: one moment, predict q , constant D_n	E: two moment, predict q , predict D_n	F: two moment, predict q , predict N_t
$q (\times 10^3)$	1.00	3.52	5.75	8.35	3.19
q RD against F (%)	—	10.34	80.25	161.76	—
$N_t (\times 10^7 \text{ m}^{-3})$	1.00	1.37	5.75	15.30	1.00
N_t RD against F (%)	—	37.0	475.08	1428.20	—
$D_n (\times 10^6 \text{ m})$	17.71	24.26	17.71	14.45	26.08
D_n RD against F (%)	—	6.99	32.1	44.48	—
$n_o [\times 10^{11} \text{ m}^{-(\beta+\nu)}]$	56.43	56.43	324.71	1055.37	38.34
n_o RD against F (%)	—	47.27	746.91	2652.69	—

$dt \approx D^\delta$ can be made with no complications to analyze scheme E for the continuous collection growth equation.

Let x be the subscript for gamma-distributed collector particles, such as graupel, and let y be the subscript for monodispersed collectee particles, such as cloud water. Assume that $D_x \gg D_y$, $V_x \gg V_y$, $V_x = aD^b$, and $m(D) = \alpha D^\beta$, where $a = [(4\rho_x g)/(3\rho_o C_{d,x})]^b$ and $b = 0.5$ (g is the gravitational acceleration, and C_d is the drag coefficient). The continuous collection growth equation integrated over $D[0, \infty]$ may be written as

$$\frac{dq_x}{dt} = \int_0^\infty \frac{\pi E_{x,y} N_x q_y D_x^2 a D_x^b}{4} n(D) dD. \quad (13)$$

From (13), the following conservation equation is obtained:

$$\frac{dq_x}{dt} = \frac{\pi E_{x,y} N_x q_y D_{n,x}^{2.5} \Gamma(2.5 + \nu_x)}{4\Gamma(\nu_x)} \left(\frac{4\rho_x g}{3\rho_o C_{d,x}} \right)^{0.5}, \quad (14)$$

along with

$$\frac{dN_{t,x}}{dt} = 0. \quad (15)$$

To evaluate the four schemes for the continuous collection growth process we specify $\beta = 3$ for a sphere, $\nu = 3$ for the distribution shape parameter, $q_x = 4 \times 10^{-3}$ kg kg⁻¹ as initial value for graupel mixing ratio, $E_{x,y} = 0.55$ for collection efficiency, $\rho_x = 900$ kg m⁻³ for density of graupel, $C_d = 0.60$ for drag coefficient for graupel in (14), $g = 9.8$ m s⁻² for gravitational acceleration, $q_y = 1.0 \times 10^{-3}$ kg kg⁻¹ as a constant value of the mixing ratio for cloud water, and $\delta = 2.5$ from (14).

Solutions are obtained for (14) and (15) by numerically integrating the continuous collection equation forward in time from 0 to 300 s using a 1-s time step. Scheme F is used for the reference solution again to

compare with the other schemes. Results are shown for integrations at $t = 300$ s in Table 3.

Overall, scheme E shows the worst performance against scheme F. The RDs against scheme F are nearly similar for schemes A and B. Not surprising is that the trends for schemes A, B, and E are very similar to those for vapor diffusion growth. Particles do not become large enough, but particles become more numerous for schemes A, B, and E as before, which violates the conservation of N_t [(15)]. All of the results are physically incorrect for D_n , N_n , and n_o , because there is no mechanism for a gain in N_t [(15)]. Only scheme F provides physically consistent solutions.

4. Conclusions

With the rapid increase in the use of microphysical parameterizations in numerical models we felt compelled to evaluate the veracity of some commonly used microphysical moment schemes in an idealized controlled manner (holding the rate of the third-moment dq/dt constant and computing other variables). It has been shown that schemes A, B, and E (Table 1), which are very often used in numerical cloud models, do not conserve the important moment N_t when they physically should do so for the processes of vapor diffusional growth and continuous collection growth (Tables 2 and 3). In particular, schemes A, B, and E all artificially nucleate or introduce particles during processes that should conserve N_t . In some of the tested cases, the characteristic diameters get smaller than initial diameter values as time increases (e.g., for scheme E) as the distribution slope awkwardly becomes more negative (larger) with time. If given a choice of schemes, such as those presented herein, the results make it possible to say which scheme really is the most physically consistent; a strong case could be made that a scheme that predicts (q, N_t) , a two-moment method (scheme F), is

TABLE 3. As in Table 2, but for continuous collection growth.

Scheme	Initial values for all schemes	Final values and errors relative to scheme F			
		A: one moment, predict q , constant n_o	B: one moment, predict q , constant D_n	E: two moment, predict q , predict D_n	F: two moment, predict q , predict N_t
q ($\times 10^3$)	1.00	4.32	4.97	5.46	4.15
q RD against F (%)	—	41.06	49.71	54.86	—
N_t ($\times 10^3$ m ⁻³)	100.00	144.13	497.12	1135.10	100.00
N_t RD against F (%)	—	26.50	397.12	1035.10	—
D_n ($\times 10^6$ m)	445.10	641.54	445.10	349.29	715.03
D_n RD against F (%)	—	10.27	37.75	51.15	—
n_o [$\times 10^6$ m ^{-($\beta+\nu$)}]	2.25	2.25	11.17	32.50	1.40
n_o RD against F (%)	—	60.64	698.60	2223.62	—

the most physically consistent and least suspect, at least for some problems for the diffusion and accretion growth processes.

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CORRIGENDUM

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Three equations contain errors in Straka et al. (2005), although they were programmed correctly for the work presented. Equation (10) should have read

$$\frac{dq}{dt} = \int_0^\infty \frac{1}{\rho_o} \frac{2\pi D f(S_x - 1)}{\left(\frac{L_s^2}{KR_v T^2} + \frac{1}{\rho_o q_{is} \varphi_v}\right)} n(D) dD; \quad (10)$$

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that is, there was an incorrect factor of N_t in the numerator. Equation (11) should have read

$$\frac{dq}{dt} = \frac{1}{\rho_o} \frac{2\pi D_n N_t f(S_x - 1)}{\left(\frac{L_s^2}{KR_v T^2} + \frac{1}{\rho_o q_{is} \varphi_v}\right)} \frac{\Gamma(1 + \nu)}{\Gamma(\nu)}; \quad (11)$$

that is, the gamma terms were omitted. Equation (13) should have read

$$\frac{dq_x}{dt} = \int_0^\infty \frac{\pi E_{x,y} q_y D_x^2 a D_x^b}{4} n(D) dD; \quad (13)$$

that is, there was an incorrect factor of N_x in the numerator. In addition, Tables 2 and 3 have been updated

TABLE 2. Results from vapor diffusion growth of an ice sphere from 0 to 300 s. In columns A–F, the top values are the 300-s values and the bottom values are the errors relative to scheme F. Relative differences (RD; percent) are based on $100 \times |(\text{true} - \text{predicted}) / \text{true}|$, where true values are from scheme F and predicted values are from the other schemes.

Scheme	Initial values for all schemes	Final values and errors relative to scheme F			
		A: one moment, predict q , constant n_o	B: one moment, predict q , constant D_n	E: two moment, predict q , predict D_n	F: two-moment, predict q , predict N_t
q ($\times 10^{-3}$)	1.00	3.13	39.86	2.67	4.97
q RD against F (%)	—	17.14	49.42	86.14	—
N_t ($\times 10^7 \text{ m}^{-3}$)	1.00	1.77	3.99	7.84	1.00
N_t RD against F (%)	—	27.56	249.94	683.87	—
D_n ($\times 10^{-6} \text{ m}$)	13.06	15.79	13.06	11.21	18.11
D_n RD against F (%)	—	12.81	27.90	38.08	—
n_o [$\times 10^{20} \text{ m}^{-(\beta+\nu)}$]	44.91	44.91	179.04	555.76	16.84
n_o RD against F (%)	—	166.78	963.44	3201.06	—

TABLE 3. As in Table 2, but for continuous collection growth.

Scheme	Initial values for all schemes	Final values and errors relative to scheme F			
		A: one moment, predict q , constant n_o	B: one moment, predict q , constant D_n	E: two moment, predict q , predict D_n	F: two moment, predict q , predict N_t
q ($\times 10^{-3}$)	4.00	8.16	8.34	8.00	8.13
q RD against F (%)	—	2.10	4.23	1.62	—
N_t (m^{-3})	1000.00	1429.46	2085.17	1332.67	1000.0
N_t RD against F (%)	—	42.95	108.52	33.27	—
D_n ($\times 10^{-6}$ m)	520.93	586.82	520.93	599.66	656.38
D_n RD against F (%)	—	10.60	20.63	8.64	—
n_o [$\times 10^{13}$ $m^{-(\beta+\nu)}$]	7.07	7.07	14.75	6.18	3.54
n_o RD against F (%)	—	100.04	317.14	74.78	—

after eliminating a computer coding error in which some of the input values correctly presented in the paper were incorrectly coded in the simple model. With the correction to the code, scheme E is the second best for collection growth instead of scheme A (but not for diffusion growth).

REFERENCES

Straka, J. M., M. S. Gilmore, K. M. Kanak, and E. N. Rasmussen, 2005: A comparison of the conservation of number concentration for the continuous collection and vapor diffusion growth equations using one- and two-moment schemes. *J. Appl. Meteor.*, **44**, 1844–1849.