

Variational Optimization Method for Calculation of Cloud Drop Growth in an Eulerian Drop-Size Framework

QINGFU LIU, YEFIM L. KOGAN, DOUGLAS K. LILLY, AND MARAT P. KHAIROUTDINOV

Cooperative Institute for Mesoscale Meteorological Studies, University of Oklahoma, Norman, Oklahoma

(Manuscript received 20 March 1996, in final form 17 March 1997)

ABSTRACT

A variational optimization (VO) method that requires specification of only one variable in each bin size for condensation and evaporation calculations in an Eulerian drop-size framework is proposed. The method is tested against the exact solution given by the Lagrangian method using more than 15 000 spectra selected from experiments with a three-dimensional large eddy simulation model with explicit microphysics. The results show that the VO method not only conserves the integral parameters of the spectrum, such as drop number, mean radius, liquid water content, and the effective radius, but also provides an accurate calculation of the spectrum itself.

1. Introduction

The current generation of cloud microphysical models that combine three-dimensional dynamics and an explicit formulation of microphysics requires an Eulerian drop-size framework in which drop sizes are fixed. The evolution of the spectra is described by varying the number concentration and/or mass within each size category. As a result of the drop growth processes, such as condensation, evaporation, coagulation, etc., new size categories will form that need to be remapped to the Eulerian fixed bin sizes at the end of each time step. It is during the remapping procedure that the added mass in the case of condensation (or number concentration in the case of coagulation) is usually spread over the entire bin size interval, resulting in numerical dispersion of the spectra. The numerical dispersion, to a certain degree unavoidable in any Eulerian formulation, if excessive, can result in broadening of the cloud drop spectrum and acceleration of the collection process, thus leading to an earlier development of precipitation. In a similar manner, it may accelerate the evaporation of cloud drops in the descending branches of cloud circulation.

The development of numerical methods for accurate calculation of cloud drop growth in an Eulerian drop-size framework has been the subject of many studies (e.g., Kovetz and Olund 1969; Bleck 1970; Egan and Mahoney 1972; Berry and Reinhardt 1974; Young 1974; Ochs and Yao 1978; Tzivion et al. 1987). A simple and

computationally efficient method that conserves both the mass and number concentration has been proposed by Kovetz and Olund (1969) (hereafter referred to as KO). In essence, the KO method represents the first-order upwind advection algorithm and results in large numerical diffusion. However, due to its simplicity, the method has been applied both to condensational and coagulation growth calculations. In coagulation calculation, as shown by Ochs and Yao (1978), the large numerical dispersion of the method results in artificial production of precipitation. As we will show later in this paper, the KO method gives also quite inaccurate solutions for droplet condensational growth under conditions typical for stratocumulus cloud layers.

A much more accurate method has been developed by Egan and Mahoney (1972) (referred hereafter as EM). This method conserves the zero (drop concentration), first (liquid water content), and second (radar reflectivity) moments of a drop mass distribution. Later, Ochs and Yao (1978) extended the technique to a non-uniform exponential mass coordinate and applied it for collection and breakup, as well as for condensation calculations. Young (1974) proposed a numerical method using separate number and mass conservation equations, thus allowing subbin resolution. Both EM and Young's methods provide much more accurate solutions than single-moment schemes and have been successfully used in models with simplified dynamic frameworks. It has to be noted, however, that the use of higher moments of the distribution function increases the number of microphysical variables that need to be retained in the EM method by a factor of 3 and, in Young's method, by a factor of 2. In multidimensional models, the computational burden of these methods is quite significant.

Corresponding author address: Qingfu Liu, CIMMS, University of Oklahoma, 100 E. Boyd, Norman, OK 73019.
E-mail: qliu@tornado.ou.edu

Liu et al. (1995) described a variational optimization (VO) method that requires specification of only one variable in each bin size. The method significantly limits the numerical dispersion and can be formulated to conserve arbitrary number of moments of the drop-size distribution. It is also computationally inexpensive and can be easily incorporated in multidimensional cloud models. In the present paper we provide a detailed description of the method and describe modifications of the algorithm for the case of precipitating clouds. The accuracy of the method is tested using more than 15 000 cloud drop spectra generated by the three-dimensional large eddy simulation (LES) cloud model with explicit microphysics (Kogan et al. 1995).

2. Formulation of the method

The variational methods, first applied in meteorology by Sasaki (1958), have become powerful tools in optimization, numerical analysis, and data assimilation (e.g., Lewis 1972; Stephens 1970; Ritchie 1975). In this paper, we apply a variational method for remapping the drop-size distribution function during calculations of condensational growth in an Eulerian drop-size framework. In the latter, the evolution of a drop spectrum is represented by the changing concentration of drops within the fixed size bins. The variational method controls the numerical dispersion by imposing the moment-conserving constraints. In the following discussion, we denote the drop radius in each stationary bin as r_i ($i = 1, 2, \dots, K$) assuming for convenience $r_1 < r_2 < \dots < r_K$. Let us consider a distribution of which the cloud droplet number is N_i^* in bin i . As condensation occurs, the drop radius in i th category grows from r_i to r_i^* . Our goal is to find the new drop numbers in each stationary bin.

We start with the first guess of a spectrum, which is obtained by the KO method. The first guess conserves the total number of cloud drops and the total liquid water content.

Now, we define the cost function in the form

$$J = \frac{1}{2} \sum_{i=1}^K w_i (N_i - \tilde{N}_i)^2, \tag{1}$$

subject to the strong constraints

$$\sum_{i=1}^K N_i = C, \tag{2}$$

$$\sum_{i=1}^K N_i r_i = R, \tag{3}$$

$$\sum_{i=1}^K N_i r_i^2 = S, \tag{4}$$

$$\sum_{i=1}^K N_i r_i^3 = Q, \tag{5}$$

where w_i are the weights ($w_i > 0$) defined later in this

section. Here, \tilde{N}_i is the cloud drop number in category i of the first guess and N_i is the sought-after new cloud drop number concentration. The new spectrum (r_i, N_i) conserves the zero, first, second, and third moments of the distribution (r_i^*, N_i^*) , which represent the total droplet number, mean droplet radius, total droplet surface area, and the total liquid water content (hence the effective radius is also conserved). The zero (C), first (R), second (S), and the third moments (Q), of the distribution (r_i^*, N_i^*) are defined as

$$\begin{aligned} C &= \sum_{i=1}^K N_i^* & R &= \sum_{i=1}^K N_i^* r_i^* \\ S &= \sum_{i=1}^K N_i^* (r_i^*)^2 & Q &= \sum_{i=1}^K N_i^* (r_i^*)^3. \end{aligned}$$

By requiring the minimum of the cost function through the use of Lagrangian function L and Lagrangian multipliers $\lambda_1, \lambda_2, \lambda_3$, and λ_4 ,

$$\begin{aligned} L &= \frac{1}{2} \sum_{i=1}^K w_i (N_i - \tilde{N}_i)^2 + \lambda_1 \left(\sum_{i=1}^K N_i - C \right) \\ &+ \lambda_2 \left(\sum_{i=1}^K N_i r_i - R \right) + \lambda_3 \left(\sum_{i=1}^K N_i r_i^2 - S \right) \\ &+ \lambda_4 \left(\sum_{i=1}^K N_i r_i^3 - Q \right), \end{aligned}$$

one can obtain

$$w_i (N_i - \tilde{N}_i) + \lambda_1 + \lambda_2 r_i + \lambda_3 r_i^2 + \lambda_4 r_i^3 = 0. \tag{6}$$

Solving for N_i from Eq. (6),

$$N_i = \tilde{N}_i - \frac{1}{w_i} (\lambda_1 + \lambda_2 r_i + \lambda_3 r_i^2 + \lambda_4 r_i^3), \tag{7}$$

and substituting Eq. (7) into Eq. (2), (3), (4), and (5), we obtain four equations for four unknowns $\lambda_1, \lambda_2, \lambda_3$, and λ_4 that give

$$\lambda_1 = \frac{\Delta_1}{\Delta}, \quad \lambda_2 = \frac{\Delta_2}{\Delta}, \quad \lambda_3 = \frac{\Delta_3}{\Delta}, \quad \lambda_4 = \frac{\Delta_4}{\Delta}, \tag{8}$$

where

$$\begin{aligned} \Delta &= \begin{vmatrix} a_1 & b_1 & c_1 & d_1 \\ a_2 & b_2 & c_2 & d_2 \\ a_3 & b_3 & c_3 & d_3 \\ a_4 & b_4 & c_4 & d_4 \end{vmatrix}, \\ \Delta_1 &= \begin{vmatrix} \Delta C & b_1 & c_1 & d_1 \\ \Delta R & b_2 & c_2 & d_2 \\ \Delta S & b_3 & c_3 & d_3 \\ \Delta Q & b_4 & c_4 & d_4 \end{vmatrix}, & \Delta_2 &= \begin{vmatrix} a_1 & \Delta C & c_1 & d_1 \\ a_2 & \Delta R & c_2 & d_2 \\ a_3 & \Delta S & c_3 & d_3 \\ a_4 & \Delta Q & c_4 & d_4 \end{vmatrix}, \end{aligned}$$

$$\Delta_3 = \begin{vmatrix} a_1 & b_1 & \Delta C & d_1 \\ a_2 & b_2 & \Delta R & d_2 \\ a_3 & b_3 & \Delta S & d_3 \\ a_4 & b_4 & \Delta Q & d_4 \end{vmatrix}, \quad \Delta_4 = \begin{vmatrix} a_1 & b_1 & c_1 & \Delta C \\ a_2 & b_2 & c_2 & \Delta R \\ a_3 & b_3 & c_3 & \Delta S \\ a_4 & b_4 & c_4 & \Delta Q \end{vmatrix},$$

and

$$a_1 = \sum_{i=1}^K \frac{1}{w_i}, \quad b_1 = \sum_{i=1}^K \frac{r_i}{w_i}, \quad c_1 = \sum_{i=1}^K \frac{r_i^2}{w_i}, \quad d_1 = \sum_{i=1}^K \frac{r_i^3}{w_i},$$

$$a_2 = b_1, \quad b_2 = c_1, \quad c_2 = d_1, \quad d_2 = \sum_{i=1}^K \frac{r_i^4}{w_i},$$

$$a_3 = c_1, \quad b_3 = d_1, \quad c_3 = d_2, \quad d_3 = \sum_{i=1}^K \frac{r_i^5}{w_i},$$

$$a_4 = d_1, \quad b_4 = d_2, \quad c_4 = d_3, \quad d_4 = \sum_{i=1}^K \frac{r_i^6}{w_i},$$

$$\Delta C = \sum_{i=1}^K \tilde{N}_i - C, \quad \Delta R = \sum_{i=1}^K \tilde{N}_i r_i - R,$$

$$\Delta S = \sum_{i=1}^K \tilde{N}_i r_i^2 - S, \quad \Delta Q = \sum_{i=1}^K \tilde{N}_i r_i^3 - Q.$$

In a very few cases, the determinant Δ may become very small ($< 10^{-7} \sim 10^{-8}$), for example, when the spectrum is very narrow (say cloud drops only spread over less than four bins). In this case, we simply use the KO method without the variational adjustment (see appendix A). Otherwise, we can solve for $\lambda_1, \lambda_2, \lambda_3,$ and λ_4 and then calculate the adjusted cloud droplet number for each bin i using Eq. (7).

Variational optimization technique does not impose constraints on the determination of weights (w_i) in the cost function. In most variational optimization problems the weights are chosen empirically based on the specifics of the problem. Liu et al. (1995) give the weights as $w_i = \tilde{N}_i^{-\gamma}$, where $\gamma = 1.0$. A series of numerical tests using a Lagrangian air parcel model that provides an exact solution of the condensation problem showed that this weight function works very well in the case of nonprecipitating clouds. However, in the case of precipitating stratocumulus or convective clouds, where the cloud drop size range covers hundreds and even thousands microns, much better results are obtained by the weights in the form $w_i = \tilde{N}_i / (1 + (r_i/\beta)^3)$, where $\beta = 10 \mu\text{m}$. Our tests showed that this weight function works equally well in the case of nonprecipitating clouds.

3. Description of the Lagrangian air parcel model

The Lagrangian air parcel model used in our tests follows that of Kornfeld (1970). We consider an air parcel that contains dry air, water vapor, and cloud drops and is rising adiabatically. The heat balance equation during the moist-adiabatic process (see Byers 1965) is

$$-LdG_v - sG_w dT = (G_a + G_v)[C_p dT - R_v T d \ln(p)].$$

Here L is the latent heat of vaporization and s is the specific heat of water. The symbols $G_a, G_v,$ and G_w are the mass of dry air, water vapor, and liquid water in the air parcel, respectively. Here T and p are the temperature and pressure of the air parcel, respectively. Also, C_p is the specific heat of dry air at constant pressure. The specific gas constant for moist air, R_v , is given by

$$R_v = (1 + 0.608w)R_a,$$

where R_a is the specific gas constant for dry air and $w = G_v/G_a$ is the water vapor mixing ratio.

Combining the heat balance equation, the equation of state for the moist air $p = \rho R_v T$, and the hydrostatic equation $dp/dz = -\rho(g + du/dt)$, one obtains

$$\frac{dT}{dt} = \frac{-(G_a + G_v)(g + du/dt)u - L(dG_v/dt)}{(G_a + G_v)C_p + sG_w}, \quad (9)$$

$$\frac{dp}{dt} = \frac{-p(g + du/dt)u}{R_v T}, \quad (10)$$

where $u = dz/dt$ is the vertical velocity of the air parcel.

Since $G_v + G_w$ is conserved during the moist adiabatic process, we have

$$-\frac{dG_v}{dt} = \frac{dG_w}{dt} = \sum_i N_i \frac{dm_i}{dt}, \quad (11)$$

where dm_i/dt is the condensational diffusion growth rate for a cloud drop with the mass m_i in bin i , which, after neglecting both the curvature and the salt factor, can be written as (Houze 1993)

$$\frac{dm_i}{dt} = \frac{4\pi r_i f_v \tilde{S}}{F_K + F_D}. \quad (12)$$

Here F_K and F_D represent the effects of heat conductivity and the vapor diffusivity, respectively; f_v is the ventilation factor; \tilde{S} is the supersaturation, which is defined as $\tilde{S} \equiv e/e_s(T) - 1$, where e is the ambient vapor pressure and can be calculated as $e = pw/(0.622 + w)$; and $e_s(T)$ is the saturation vapor pressure given as (Murray 1967)

$$e_s(T) = 6.1078 \exp\left[\frac{17.2694(T - 273.16)}{T - 35.86}\right].$$

The set of Eqs. (9)–(12) can be solved very accurately numerically in a Lagrangian drop-size framework and provides the benchmark (exact) solution of the condensation process. The solutions of the KO, EM, and VO schemes are obtained by remapping the drop spectrum to the Eulerian drop size framework at every time step, therefore they are subject to numerical diffusion errors.

4. Verification of the method in a Lagrangian model

We first show results of the test of the VO method in a Lagrangian air parcel model. A Gamma-type dis-

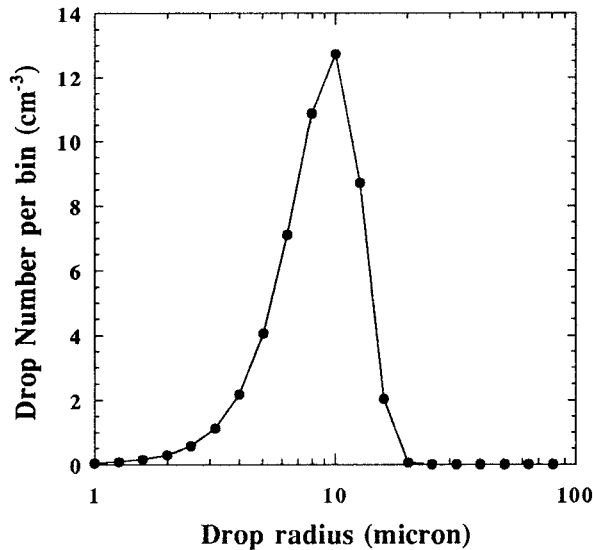


FIG. 1. Initial cloud drop spectrum used in the first two sets of experiments. The spectrum is assumed to be a Gamma distribution with liquid water content 0.2 g m^{-3} and cloud drop concentration 50 cm^{-3} .

tribution is specified initially (Berry 1967) with the liquid water content of 0.2 g m^{-3} and drop concentration of 50 cm^{-3} (Fig. 1). The stationary bin sizes are defined as $r_i = r_1 \exp[(i - 1)/I_0]$, ($i = 1, 2, \dots, 25$) with $I_0 = 3/\ln 2$. The bin sizes cover the range from $r_1 = 1$ to $256 \mu\text{m}$ and are the same as in the Cooperative Institute for Mesoscale Meteorological Studies (CIMMS) large eddy simulation (LES) cloud model (Kogan et al. 1995).

The accuracy of the VO method was evaluated in two sets of experiments, in which only condensation and evaporation processes were considered. In the first test, the air parcel ascended with a constant vertical velocity of 1.0 m s^{-1} . The drop spectra were computed using three different methods: Kovetz and Olund (1969), Egan and Mahoney (1972), and the present variational optimization method. All three methods employ an Eulerian drop-size framework. The initial supersaturation is set to be 0.2%. Figures 2a and 2b show the resulting size distribution of drop number and mass at the 200-m height. The exact solution obtained in a Lagrangian model is plotted as the solid line. As evident from Figs. 2a, 2b, and 2f, the KO method has a significant numerical dispersion, while the EM scheme has a relatively small numerical dispersion error. Since all three schemes conserve drop number and mass, the liquid water content (Fig. 2c) is determined rather accurately in all three methods. The other moments of the distribution function, such as the mean and effective radius and standard deviation, are more accurately calculated by the EM and VO schemes. The VO method produces the smallest error not only in the prediction of the integral parameters of the spectrum, such as liquid water content, mean radius, effective radius, and the relative

standard deviation of the spectrum (Figs. 2c–f), but also for the spectrum itself (Figs. 2a and 2b).

In the second set of experiments, the performance of various methods was evaluated both for condensation and evaporation processes. For this purpose, we follow an air parcel in both ascending and descending branches of its trajectory by specifying the vertical velocity variation according to the formula

$$u = u_1 + u_2 \sin(\omega t), \quad (13)$$

with $u_1 = 0$, $u_2 = 1 \text{ m s}^{-1}$ and $\omega = (2\pi/600) \text{ s}^{-1}$. The integration is made for 600 s during which time the air parcel first moves upward, reaching a height of about 191 m, and then moves downward to the same starting point, thus completing a cycle. Figures 3a and 3b show the size distribution of drop concentration and liquid water content (LWC) in the air parcel at the end of the cycle. The results are remarkably good for both the EM and VO schemes, which both preserve well the spectrum shape. The EM scheme does exhibit a moderate dispersion, while the VO method has a small phase error. The KO method shows a very significant dispersion (largest in both diffusion and phase error). Due to the strong dispersion, the KO method results in evaporation of a significant number of cloud drops (58%). Only a small fraction (less than 4%) of cloud drops evaporates in the VO scheme (Fig. 3c).

5. Modification of the VO method for precipitating clouds

The VO method has been implemented in the CIMMS LES model with explicit microphysics (Kogan et al. 1995). The three-dimensional experiments showed that the method works very well in simulations of nonprecipitating stratocumulus clouds. Since coalescence is weak in these clouds, the cloud drop spectra are mostly unimodal and occupy a rather limited size range from 1 to 50 microns in radius. The situation is more complex in the case of precipitating clouds where bimodal drop-size distributions are quite common. In this case, the constraints to conserve four moments of the drop distribution imposed by the VO method may lead to artificial reduction in the drop concentration at the tails of the spectrum. The right “large-droplet” tail of the spectrum is especially important as it determines the onset of coagulation and also rain and drizzle formation rates.

The problem can be effectively solved and the concentration of drops at the spectrum tails preserved by applying the VO method to the central part of the drop spectrum and to each of its tails separately. The decomposition of the spectrum into three subspectra produces the smallest error when the subspectra are smooth and do not have sharp discontinuities. This can be achieved by using Gamma distribution function in the decomposition procedure described in appendix B and illustrated conceptually in Fig. 4.

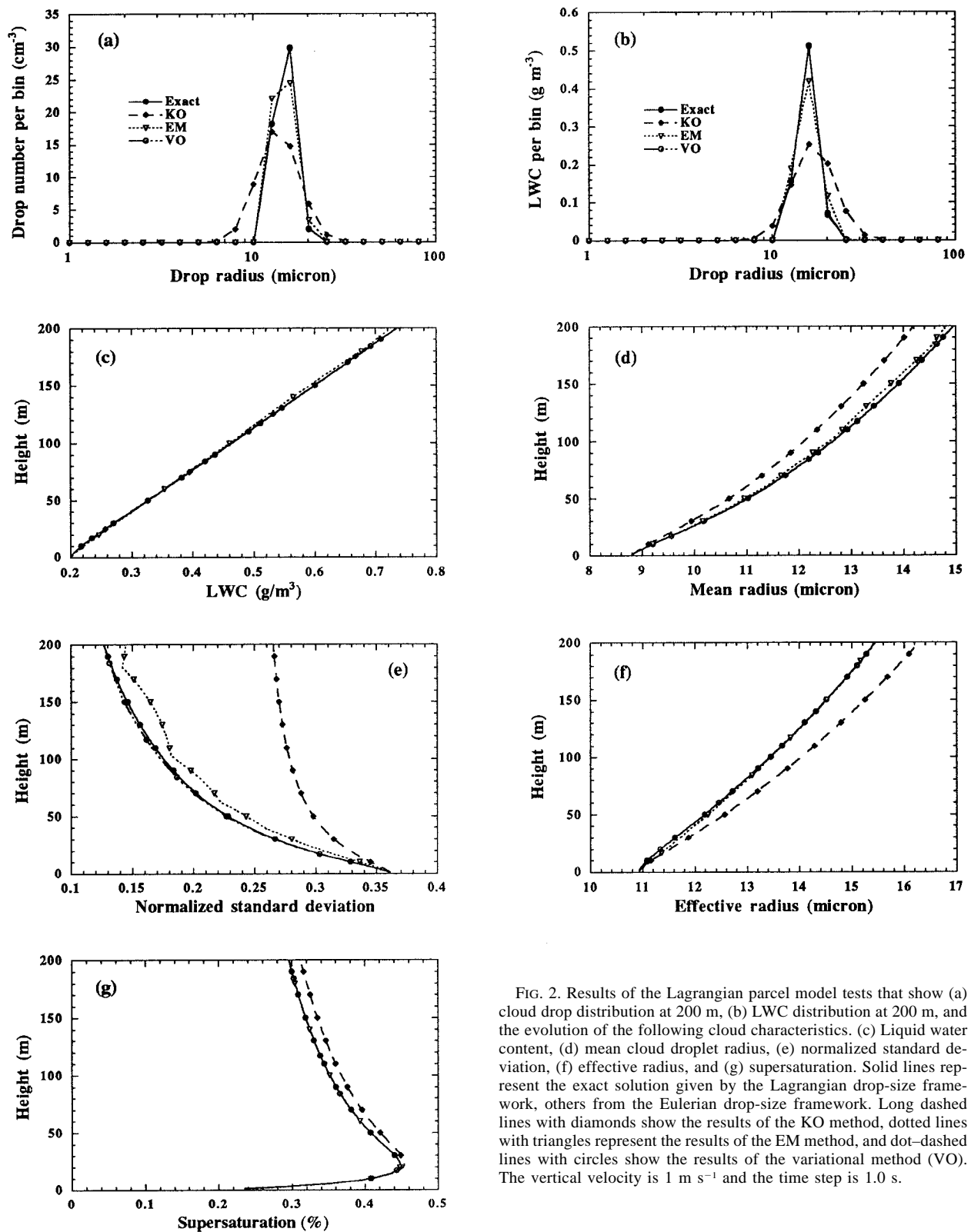


FIG. 2. Results of the Lagrangian parcel model tests that show (a) cloud drop distribution at 200 m, (b) LWC distribution at 200 m, and the evolution of the following cloud characteristics. (c) Liquid water content, (d) mean cloud droplet radius, (e) normalized standard deviation, (f) effective radius, and (g) supersaturation. Solid lines represent the exact solution given by the Lagrangian drop-size framework, others from the Eulerian drop-size framework. Long dashed lines with diamonds show the results of the KO method, dotted lines with triangles represent the results of the EM method, and dot-dashed lines with circles show the results of the variational method (VO). The vertical velocity is 1 m s^{-1} and the time step is 1.0 s.

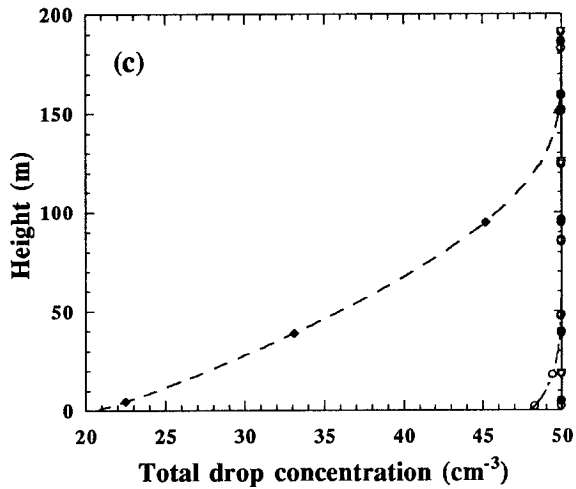
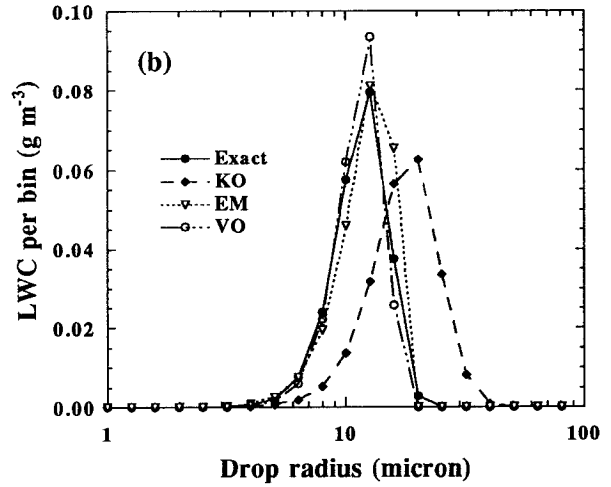
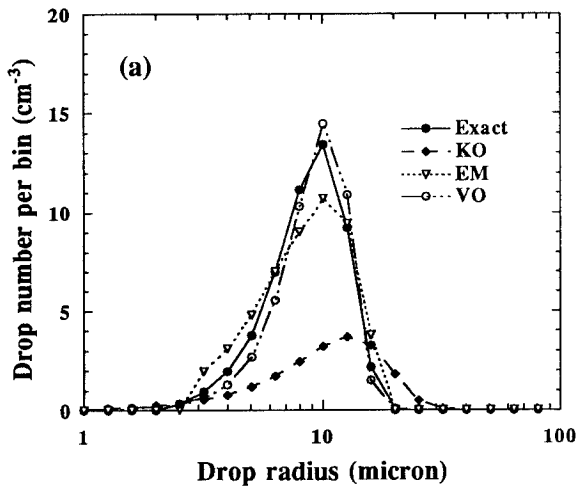


FIG. 3. The effects of condensation and evaporation on (a) cloud drop number spectrum, (b) LWC spectrum, and (c) total cloud drop concentration after the air parcel goes up and down, returning to the starting point. The notations are the same as in Fig. 2.

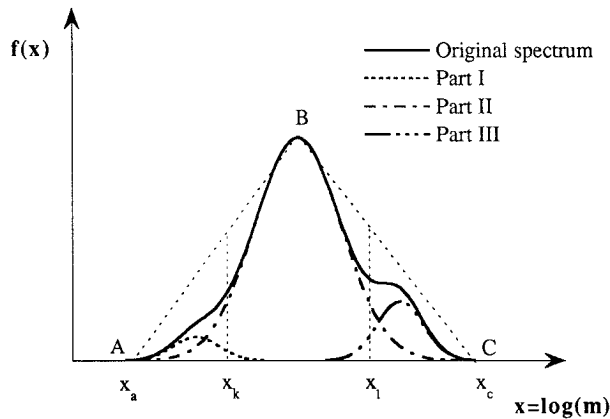


FIG. 4. The conceptual model illustrating the decomposition procedure described in appendix B. Here $f(x)$ denotes the LWC per bin and x is the logarithm of cloud drop mass m .

The VO method modified for precipitation clouds was tested in a two different sets of experiments. The first set used two typical spectra produced as a result of the coalescence process and characterized by the long large-drop tail and double peaks in the LWC distribution. The spectra were obtained using Berry and Reinhardt (1974) coalescence model that was initialized with a Gamma-type drop distribution with LWC of 1.0 g m^{-3} and cloud drop concentration of 50 cm^{-3} . The coalescence model was run for 316 and 476 s, respectively, to obtain the spectra 1 and 2 shown in Figs. 5a and 5b. Figures 5a and 5b also show the decomposition of the two spectra into three parts. The spectra 1 and 2 shown in Figs. 5a and 5b were then used as the input spectra for the Lagrangian condensation parcel model and run for another 500 time steps with a constant vertical velocity of 1.0

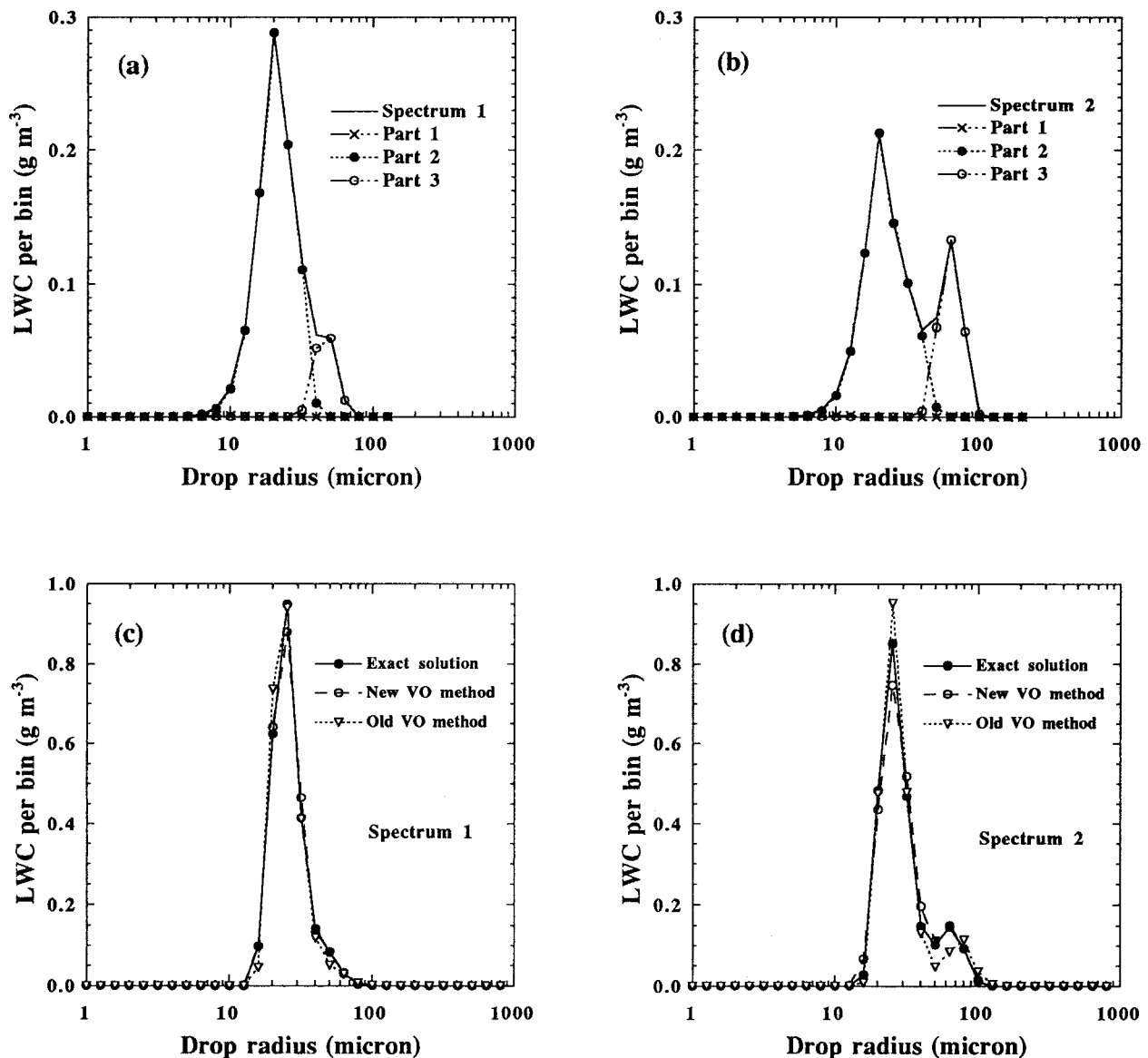


FIG. 5. Two typical spectra produced by coalescence model and the results from Lagrangian parcel model tests. (a) and (b) The LWC spectra and their decompositions into three parts for spectrum I (long large-drop tail) and spectrum II (bimode distribution), respectively. (c) and (d) The averaged solution and errors from Lagrangian parcel model tests at 500 time steps for spectrum I and spectrum II, respectively. In this set of experiments, the vertical velocity is 1 m s^{-1} and the time step is 1.0 s.

m s^{-1} . As in the experiments described in section 3, the exact solution of the Lagrangian condensation model is then compared to the solution given by the VO method in the Eulerian framework. The present experiments, however, use spectrum 1 and 2 that have a significant drizzle mode compared to initial spectrum shown in Fig. 1. The results of the experiments are shown in Figs. 5c and 5d (note the difference in scales in Fig. 5 due to the increase in LWC as a result of condensation). The modified VO method that uses the decomposition procedure provides more accurate solution than the old version of the VO method, especially for the large-drop tail of the spectra. The increased accuracy in this size

range is especially important for drizzle and rain prediction in precipitating clouds.

The tests of the method so far used a rather limited set of spectra. In the second set of experiments, we used a much wider variety of spectra obtained under a broad range of dynamic conditions typical for stratocumulus clouds. These spectra were produced by a three-dimensional LES model initialized with the dataset obtained by Nicholls during the field experiment conducted in the Northern Atlantic (Nicholls 1984). The case study based on this dataset is described in Kogan et al. (1995) and showed reasonably good agreement between the LES model-predicted microphysics and observations.

TABLE 1. Classification of the cloud drop spectra.

Group	Radar reflectivity range (cm ⁶)	Total number of spectra	Comment
I	0 ~ 10 ⁻¹⁷	4472	Unimodal spectra
II	10 ⁻¹⁷ ~ 10 ⁻¹⁶	9512	Long tail in the drizzle range
III	10 ⁻¹⁶ ~ 4 · 10 ⁻¹⁶	1048	Small second peak in the drizzle range
IV	> 4 · 10 ⁻¹⁶	268	Double peaks of comparable magnitude
	Total:	15 300	

The model simulation provided us with more than 15 000 spectra, which comprised the dataset with LWC in the range of 0.1–0.5 g m⁻³ and drop concentrations in the range of 30–90 cm⁻³. The whole dataset was divided into four groups based on the radar reflectivity parameter

$$Z = \frac{\sum_i N_i r_i^6}{\sum_i N_i}.$$

The latter parameter allows us to separate the dataset into groups with different values of LWC in the drizzle mode size range. The classification of the spectra is summarized in Table 1. The average spectra and the standard deviation of the spectra in each group are shown in Figs. 6a, 6b, 7a, and 7b.

Each of the 15 300 spectra was tested in the Lagrangian parcel model described in section 3. The vertical velocity of the air parcel was specified according to (9) with $w_1 = 0.25$ m s⁻¹, $w_2 = 0.5$ m s⁻¹, and $\omega = (\pi/20)$ s⁻¹. The resulting spectra of the modified VO method are then compared to the exact solutions after 600 time steps. We calculated the averaged difference (error) ε_i between the solution given by the VO method N_i^j and the corresponding exact Lagrangian solution \tilde{N}_i^j as

$$\varepsilon_i = \frac{1}{K} \sum_{j=1}^K |(N_i^j - \tilde{N}_i^j)| m_i, \quad (14)$$

where K is the total number of spectra in each of the four groups, i denotes the spectrum bin size, and j denotes the individual spectrum in each of the four groups described in Table 1.

Figures 6c, 6d, 7c, and 7d show the exact and the VO method solutions, as well as the error averaged over all spectra in each of the four groups. One can see that the errors are quite small and the VO method provides very satisfactory results; the improvement is especially noticeable in the drizzle size range.

Another way to evaluate the numerical diffusion of the VO method is to compare the relative dispersion of the spectrum that is defined as $\sigma_r = \sigma/\bar{r}$, where \bar{r} is the mean radius and σ is the standard variance of the spectrum,

$$\sigma = \int_0^\infty (r - \bar{r})^2 n(r) dr.$$

Table 2 lists the relative dispersion averaged over all

spectra in each of the four groups. The results show that small numerical dispersion still exists, and, in general, it increases with the broadness of the spectrum. However, even for the broadest spectra in our experiments (groups III and IV), the dispersion error is less than 10%. We would like also to note that the present tests were made using a rather coarse resolution in the drop-size coordinate where drop mass doubled every second category. It is our believe that the current generation of computers makes it quite practical to use the finer resolutions of drop spectra with mass doubling every third category. The accuracy of the VO method in this case can be increased even further.

6. Conclusions

A variational optimization method¹ for condensation and evaporation calculations in an Eulerian drop-size framework has been proposed and tested against the exact solution given by the Lagrangian air parcel model. The variational method not only conserves the integral parameters of the spectrum, such as drop number, mean radius, mass, and the effective radius, but also provides an accurate calculation of the spectrum itself. The accuracy of the variational method is comparable to the accuracy of the Egan and Mahoney (1972) scheme. The variational method has, however, an important advantage compared to the latter method. It requires specification of only one variable in each bin size, while the EM scheme needs retaining of the three moments of the spectrum, thus tripling the memory requirements in the model. For multidimensional models, this presents a serious limitation and makes the application of EM method impractical.

The estimate of computation time showed that the VO method by itself is about 3.1 times slower than the KO method. However, one has to bear in mind that 1) the remapping in a full multidimensional model needs to be done only once during the dynamical time step, and 2) the cost of the remapping is only a small fraction compared to the computational cost of other processes, such as the advection of microphysical variables, etc.

¹ The FORTRAN code of the variational optimization method can be obtained by sending a request to the leading author by e-mail at qliu@tornado.ou.edu.

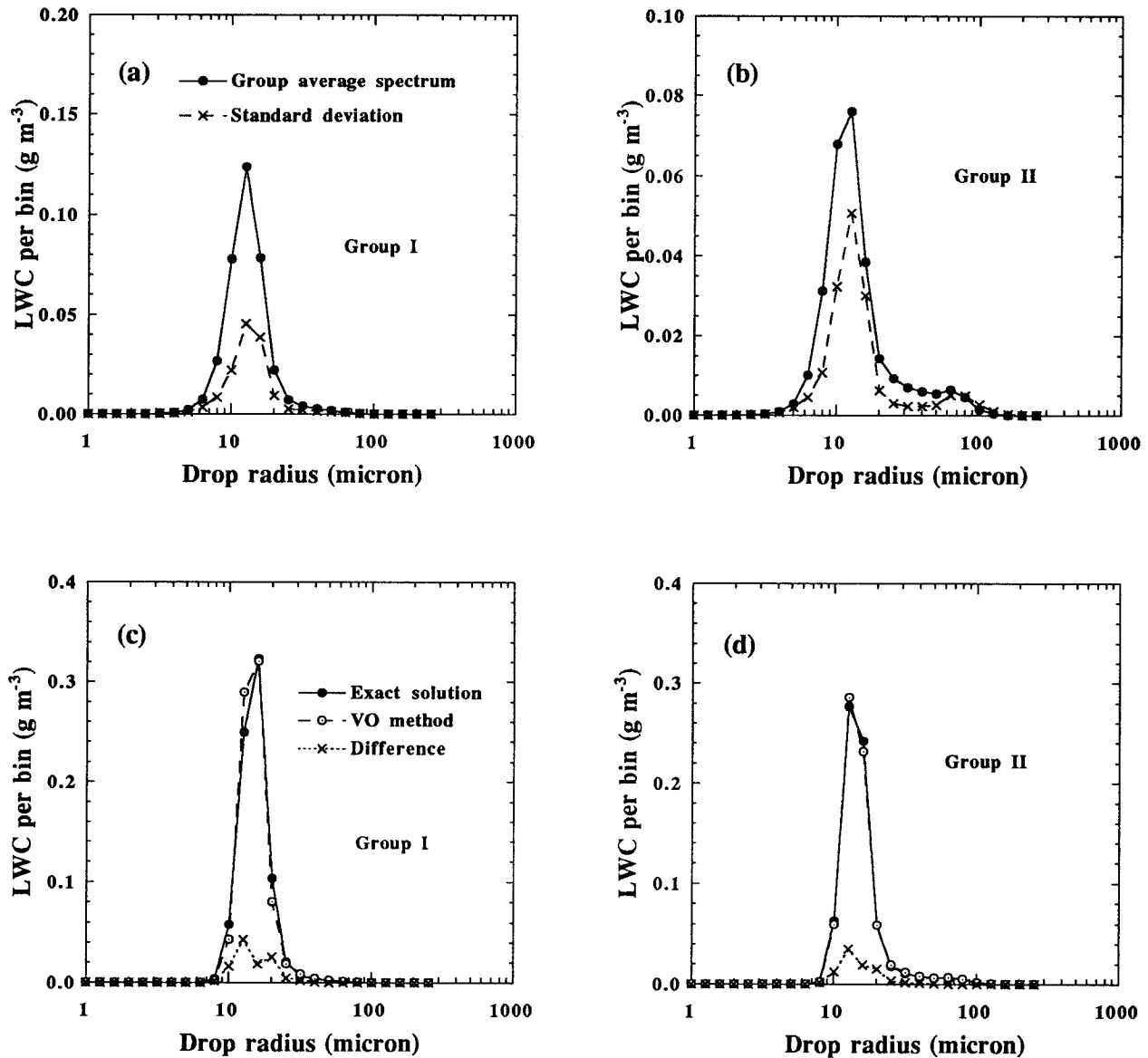


FIG. 6. Selected spectra from 3D LES model experiments and the results from Lagrangian parcel model tests. (a) and (b) The group averaged spectra and their standard deviations for group I and II, respectively. (c) and (d) The averaged solution and errors from the Lagrangian parcel model tests at 600 time steps for group I and group II, respectively. In this set of experiments, the maximum vertical velocity is 0.75 m s^{-1} and the time step is 1.0 s.

Tests with the CIMMS LES model in a $64 \times 64 \times 60$ integration domain showed that the old VO scheme for nonprecipitating clouds (Liu et al. 1995) increased the total CPU time by 1.1%, while the present version of the VO scheme for precipitating clouds increased the

total CPU time by 4.5%. Evidently this CPU time expense is justified given the significant increase in accuracy.

We would like to note that the errors associated with condensational remapping are most significant in the size range of 1–200 μm , which is typical for drops in stratiform clouds. The application of the VO method for this type of cloud is recommended. In the convective clouds where the drop-size range is much wider and the drop spectra sometimes exhibit very complex multimodal shapes, the performance of the VO method has not been thoroughly tested. However, we do expect a good performance of the VO method in convective

TABLE 2. Averaged standard deviation.

Group	Exact solution	VO method
I	0.205	0.189
II	0.203	0.206
III	0.200	0.216
IV	0.197	0.217

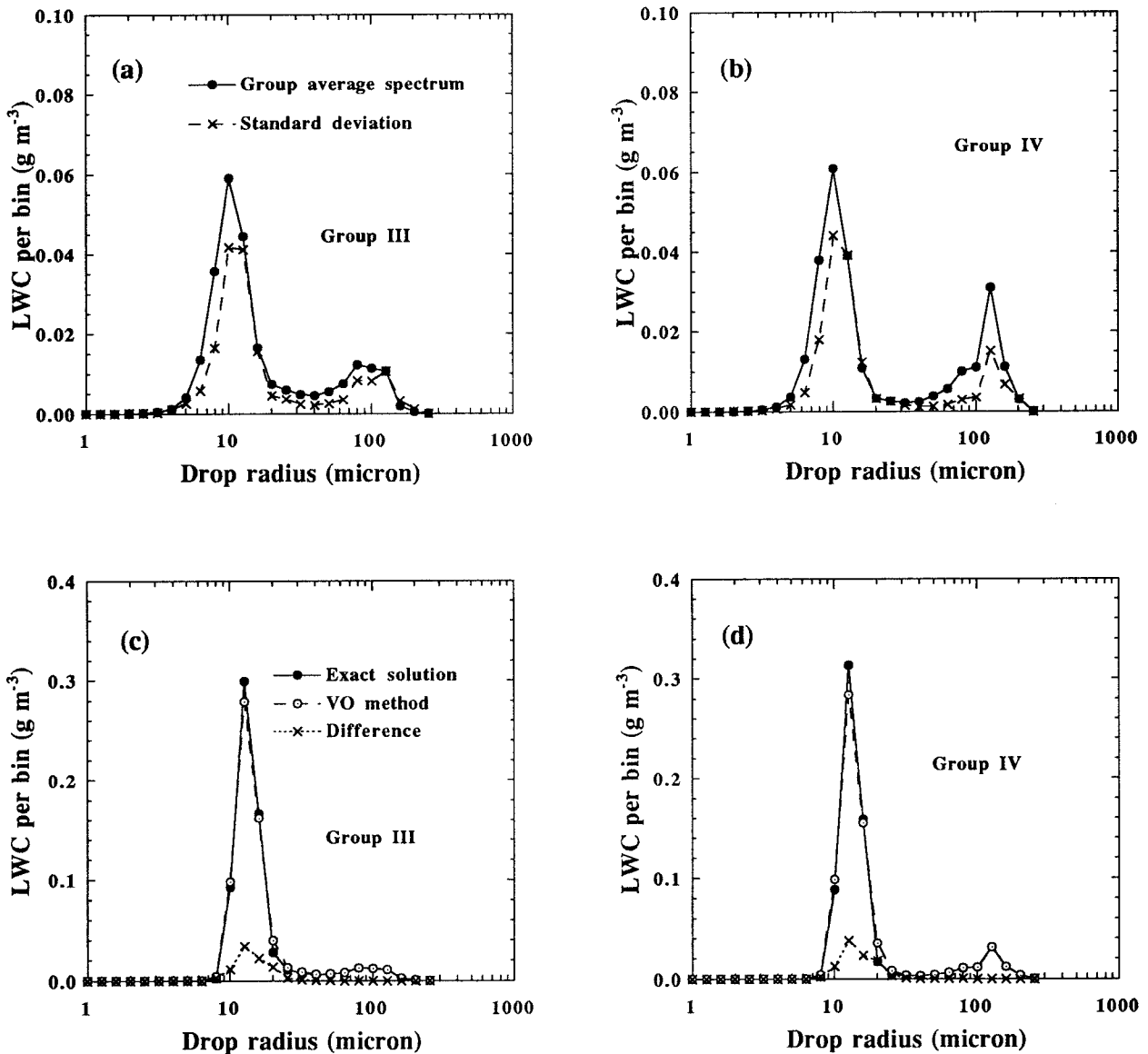


FIG. 7. As in Fig. 6 except for spectrum III and IV.

cloud models as well for two reasons. First, for large cloud drops ($r \geq 200 \mu\text{m}$) the growth by condensation is very small ($\Delta r \ll r$), therefore the condensational remapping is rather insensitive to a particular scheme. In addition, for drops larger than 100–200 μm , the condensational growth is much smaller than the coalescence growth, consequently, the errors of the condensational remapping are also smaller than the errors associated with the coagulation calculations. It is our experience that for drops larger than 100 microns, the use of a simpler method, such as Kovetz and Olund's (1969) method, is quite warranted.

Acknowledgments. The first author wishes to thank Prof. C. Qiou and Dr. Z. Wang for helpful discussions.

Support for this research was provided by the DOE ARM Project 144880-A91, the DOD-ONR Grants N00014-96-1-1112 and N00014-96-0687, the NOAA's Climate and Global Change Program Grants NA37RJ0203 and NA67RJ0150, and the NSF Grant ATM88-09862 to CAPS. Computations were performed on the DEC Alfa workstation funded by the NASA Earth Science and Application Division, Radiation Dynamic and Hydrology Branch, through Task 460-23-54-20.

APPENDIX A

Adjustment of Negative Values

As noted in Liu et al. (1995), the method may produce some small negative values in cloud drop concentration

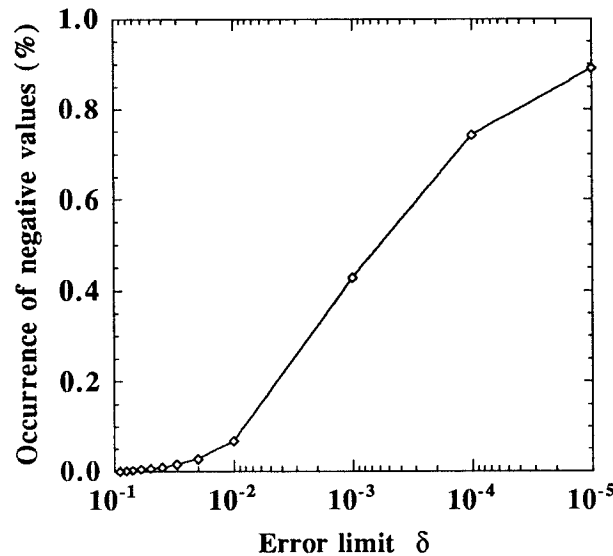


FIG. A1. Percentage occurrence of the negative values in CIMMS LES model as a function of the error limit.

that are normally associated with very sharp narrow spectra. We adjust these small negative values in the following way. Let us denote the summation of negative N_i as C^- and positive N_i as C^+ ($C = C^- + C^+$). After setting the negative N_i to be zero, the new N_i^{new} can be calculated as $N_i^{\text{new}} = N_i(1 + C^-/C^+)$. By doing this, we still have $\sum_{i=1}^K N_i^{\text{new}} = C$, but LWC is no longer conserved. Our tests show that the LWC error is very small in most cases, exceptions are associated with very narrow spectra occupying only 2–3 bins. Figure A1 shows the percentage of the negative value occurrence in the CIMMS LES model during the two dynamic time steps that produce 142 985 calls to the VO method subroutine. The calls that produced negative values were counted whenever $|C^-/C| > \delta$ or $|Q^-/Q| > \delta$. (Here, Q^- and Q are the total negative LWC and total LWC, respectively). The percentage of the calls that produce negative values are plotted in Fig. A1 as a function of δ . Of the 142 985 calls, there were no cases with negative values for $\delta = 0.09$ and only nine cases for $\delta = 0.05$. All the nine cases show that the spectra were at the early stage of activation in which cloud condensation nuclei were just activated and have not grown large enough and the drops concentrated in the first two or three bins. As δ decreases, the percentage of the negative values increases. Even for $\delta = 10^{-5}$ (0.001%), the occurrence of the negatives values is less than 1%. In fact, if the negative value is large, we use the KO method (which broadens the spectra) for one time step. At the next time step, the VO method is automatically selected, and the error again will be checked. If the error exceeds our criteria, the KO method will be used. This procedure can be repeated until all errors meet our criteria.

APPENDIX B

Description of the Decomposition Procedure

This appendix describes how the mass distribution function $f(x)$ is decomposed into three subspectra prior to condensation calculations (Fig. 4).

1) Find the maximum (B) of the spectrum, and the smallest x_a (A) and the largest x_c (C) bins that have liquid water content exceeding the minimum threshold (10^{-3} g m^{-3}).

2) Find the drop bins (x_k and x_l) at which the differences between $f(x)$ and their corresponding values on lines AB and BC is at their maximum.

3) Fit Gamma functions $G^{(1)}$ ($G^{(2)}$) that pass through the points $x_k + 1/2$ ($x_l - 1/2$) and have the same slopes as $f(x)$ at these points. The Gamma function is defined here as a two-parameter function,

$$G(x) = c_1 x^2 \exp(-c_2 x),$$

where c_1 and c_2 are constants and can be calculated as

$$c_2 = \frac{2}{x_{k+1/2}} - \frac{f'(x_{k+1/2})}{f(x_{k+1/2})},$$

$$c_1 = \frac{f(x_{k+1/2})}{x_{k+1/2}^2} \exp(c_2 x_{k+1/2}) \quad \text{for } G^{(1)},$$

and

$$c_2 = \frac{2}{x_{l-1/2}} - \frac{f'(x_{l-1/2})}{f(x_{l-1/2})},$$

$$c_1 = \frac{f(x_{l-1/2})}{x_{l-1/2}^2} \exp(c_2 x_{l-1/2}) \quad \text{for } G^{(2)}.$$

4) Decompose the spectrum into three parts:

$$\text{Part 1} \quad \begin{cases} \hat{N}_i^{(1)} = \max(0., \hat{N}_i^{(1)} - \Gamma_i^{(1)}) & x_i \leq x_k \\ \hat{N}_i^{(1)} = 0. & x_i > x_k; \end{cases}$$

$$\text{Part 2} \quad \begin{cases} \hat{N}_i^{(2)} = \min(\hat{N}_i, \Gamma_i^{(1)}) & x_i \leq x_k \\ \hat{N}_i^{(2)} = \hat{N}_i & x_k < x_i < x_l \\ \hat{N}_i^{(2)} = \min(\hat{N}_i, \Gamma_i^{(2)}) & x_i \geq x_l; \end{cases}$$

$$\text{Part 3} \quad \begin{cases} \hat{N}_i^{(3)} = 0. & x_i < x_l \\ \hat{N}_i^{(3)} = \max(0., \hat{N}_i - \Gamma_i^{(2)}) & x_i \geq x_l; \end{cases}$$

where \hat{N}_i is the drop concentration in bin i and Γ_i ($=G_i/m_i$) is the drop concentration for the fitted Gamma function.

5) Use the VO method for each part separately, then sum the outputs together.

REFERENCES

Berry, E. X., 1967: Cloud droplet growth by coalescence. *J. Atmos. Sci.*, **24**, 688–701.
 —, and R. L. Reinhardt, 1974: An analysis of cloud drop growth by collection: Part I. Double distributions. *J. Atmos. Sci.*, **31**, 1814–1824.

- Bleck, R., 1970: A fast, approximate method for integrating the stochastic coalescence equation. *J. Geophys. Res.*, **75** (27), 5165–5171.
- Byers, H. R., 1965: *Elements of Cloud Physics*. University of Chicago Press, 191 pp.
- Egan, B. A., and J. R. Mahoney, 1972: Numerical modeling of advection and diffusion of urban area source pollutant. *J. Appl. Meteor.*, **11**, 312–322.
- Houze, R. A., 1993: *Cloud Dynamics*. Academic Press, 573 pp.
- Kogan, Y. K., M. P. Khairoutdinov, D. K. Lilly, Z. N. Kogan, and Q. Liu, 1995: Modeling of stratocumulus cloud layers in a large eddy simulation model with explicit microphysics. *J. Atmos. Sci.*, **52**, 2923–2940.
- Kornfeld, P., 1970: Numerical solution for condensation of atmospheric vapor on soluble and insoluble nuclei. *J. Atmos. Sci.*, **27**, 256–264.
- Kovetz, A., and B. Olund, 1969: The effect of coalescence and condensation on rain formation in a cloud of finite vertical extent. *J. Atmos. Sci.*, **26**, 1060–1065.
- Lewis, J. M., 1972: An operational upper air analysis using the variational method. *Tellus*, **24**, 514–530.
- Liu, Q.-F., Y. L. Kogan, and D. K. Lilly, 1995: Reducing the numerical dispersion of the cloud droplet spectrum in condensation calculations. Preprints, *Conf. on Cloud Physics*, Dallas, TX, Amer. Meteor. Soc., 112–117.
- Murray, F. W., 1967: On the computation of saturation vapor pressure. *J. Appl. Meteor.*, **6**, 203–204.
- Nicholls, S., 1984: The dynamics of stratocumulus: Aircraft observations and comparisons with a mixed-layer model. *Quart. J. Roy. Meteor. Soc.*, **110**, 783–820.
- Ochs, H. T., and C. S. Yao, 1978: Moment-conserving techniques for microphysical computations. Part I: Numerical techniques. *J. Atmos. Sci.*, **35**, 1947–1958.
- Ritchie, A. A., 1975: A variational optimizing analysis approach to continuous data assimilation. Ph.D. dissertation, University of Oklahoma, 98 pp. [Available from OU Bizzell Library, Norman, OK 73019.]
- Sasaki, Y. K., 1958: An objective analysis based on the variational method. *J. Meteor. Soc. Japan*, **36**, 77–88.
- Stephens, J. J., 1970: Variational initialization with the balance equation. *J. Appl. Meteor.*, **9**, 732–739.
- Tzivion, S., G. Feingold, and Z. Levin, 1987: An efficient numerical solution to the stochastic collection equation. *J. Atmos. Sci.*, **44**, 3139–3149.
- Young, K. C., 1974: A numerical simulation of wintertime, orographic precipitation: Part I. Description of model microphysics and numerical techniques. *J. Atmos. Sci.*, **31**, 1735–1748.