Comments on "A New Monte-Carlo Simulation Model for the Temporal Development of Cloud Droplet Spectra"

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ABSTRACT

A Monte-Carlo model by Lapidus and Shafrir for the temporal development of cloud droplet spectra is critically examined. Modifications are suggested to improve the statistical validity of the model.

Both the original model and the modified model only approximately simulate the coalescence process. It is demonstrated that when large collection kernels, such as the Golovin collection kernel, are used both models are inadequate. However, for smaller and more realistic collection kernels the models do not produce results that differ substantially from the standard solutions given by the coalescence equations.

1. Introduction

Lapidus and Shafrir (1972) present a Monte-Carlo model for studying the temporal development of cloud droplet spectra. They demonstrate the nature of the model with two examples. The first is a simple coalescence simulation that uses geometric collection kernels. The results of these calculations are compared with calculations made using a standard integral formulation of the coalescence process based on Berry (1967). The second application explores the use of the model in simulating the accretion of water drops by a falling ice particle.

Monto-Carlo techniques appear to be very useful when other microphysical processes (such as condensation) occur at the same time as the coalescence process. Here we discuss the development of a Monte-Carlo model based on that presented by Lapidus and Shafrir (1972). We have used this model, both with a Golovin (1963) collection kernel and with the more realistic collection kernels of Klett and Davis (1973), in an attempt to assess the advantages and disadvantages of the Monte-Carlo method.

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2. Mechanics of simulation

We follow the procedure set out by Lapidus and Shafrir (1972) for the discretization of the continuous cloud droplet distribution as a function of radius. We suppose that at any step of the iteration there are n_i drops m^{-3} of radius r_i and that these are randomly distributed in space according to a uniform distribution. The collection kernel for drops of radius r_i collecting drops of (smaller) radius r_j over the time interval Δt is

$$K_{ij}=\pi(r_i+r_j)^2E_{ij}(v_i-v_j)\Delta t,$$

where E_{ij} is the collection efficiency for the two drops and v_i and v_j are the respective fall velocities. The number of drops of radius r_j collected by a single drop of radius r_i in the interval Δt may reasonably be taken to be a binomially distributed random variable with parameters n_j and K_{ij} (and thus an expected value of n_jK_{ij}).

Lapidus and Shafrir model the collection of drops of radius r_j by drops of radius r_i by randomly sampling the number N_{ij} collected by one drop and then supposing that each of the n_i drops collects the same number N_{ij} of drops of radius r_j. That is, the total number of drops of radius r_j collected by drops of radius r_i in

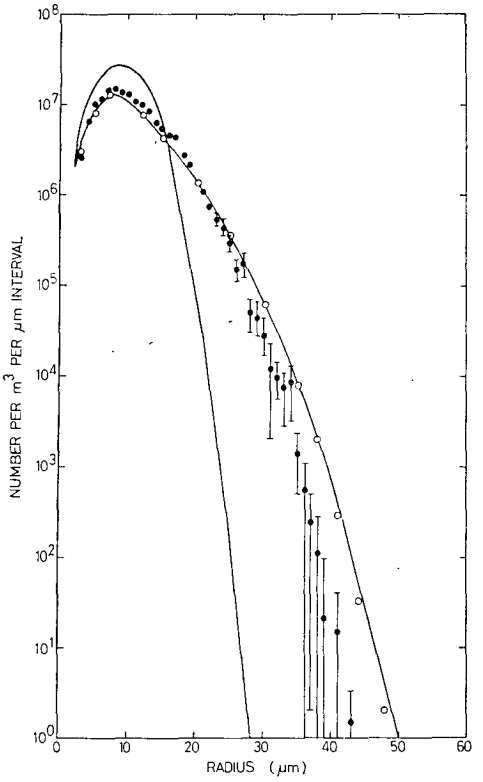

FIG. 1. The initial exponential distribution having 2.39×10^8 drops m^{-3} and the analytical solution to the coalescence equation after 400 s for the Golovin collection kernel. The open circles show the numerical solution and the closed circles the results from the Lapidus-Shafrir model. The vertical error bars show the approximate 95% confidence intervals.

interval Δt is $n_i N_{ij}$. Possible numbers collected are thus

$$0,\ n_i,\ 2n_i,\ \ldots,\ n_i n_j,$$

with respective probabilities

$$(1-K_{ij})^{n_j},\quad \binom{n_j}{1}K_{ij}(1-K_{ij})^{n_j-1},$$

$$\binom{n_j}{2}K_{ij}^2(1-K_{ij})^{n_j-2},\ \ldots,\ K_{ij}^{n_j}.$$

We have preferred to view the total number of drops collected as the sum of the numbers collected by each drop. This leads to a sum of n_i independent binomially distributed random variables, each with parameters n_j and K_{ij}. The sum, and hence the total number of drops collected, is again a binomially distributed random variable, with parameters $n_i n_j$ and K_{ij} [and expected value $n_i n_j K_{ij}$] (see Feller, 1968). Total number collected thus may be

$$0,\ 1,\ 2,\ \ldots,\ n_i n_j,$$

with respective probabilities

$$(1-K_{ij})^{n_i n_j},\quad \binom{n_i n_j}{1}K_{ij}(1-K_{ij})^{n_i n_j-1},$$

$$\binom{n_i n_j}{2}K_{ij}^2(1-K_{ij})^{n_i n_j-2},\ \ldots,\ K_{ij}^{n_i n_j}.$$

That both these formulations are approximations to reality is apparent from the observation that each provides a non-zero probability that more than the available number of drops will be indicated as having been collected. However, the model of Lapidus and Shafrir appears to assign inordinately large probabilities to the supposedly rare events when very large numbers of drops are collected. This occurs because the model, having (by random sampling) observed an unusually large number of collections by one drop, supposes the same unusual event to apply to *all* the drops of radius r_i. However, this over-representation of rare events may be somewhat suppressed by "step 5" of their procedure. In this step a check is made to see if more drops of radius r_j have been removed than are present. If such is the case, the time interval Δt is halved and another random sample taken.

Although the procedure we suggest (referred to from here on as the modified Lapidus and Shafrir model)

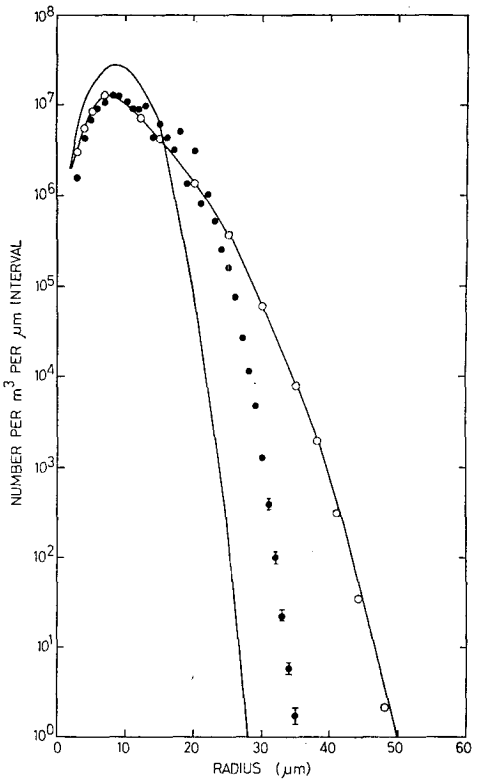

FIG. 2. As in Fig. 1 except that the closed circles show the results from the modified Lapidus-Shafrir model.

gives a more accurate picture of the total number of drops collected, it does not give any indication as to how the number of collections are distributed among the n_i drops. Since (as in the original Lapidus and Shafrir model) we distribute the mass from the collected drops evenly among all n_i drops, we overlook the occasional production of very large drops. The result is that the modified Lapidus and Shafrir model might be expected to underestimate the rate of production of large drops.

Lapidus and Shafrir (1972) have described in some detail the steps involved in their simulation procedure. However, they do not explicitly discuss the random sampling techniques they employ, other than pointing out that sampling was done with the aid of a random number generator. The details of the sampling techniques are extremely important both for the statistical validity of the model and for the efficient use of computing facilities. For these reasons we will briefly describe the sampling techniques we have used in our development of the Monte-Carlo method.

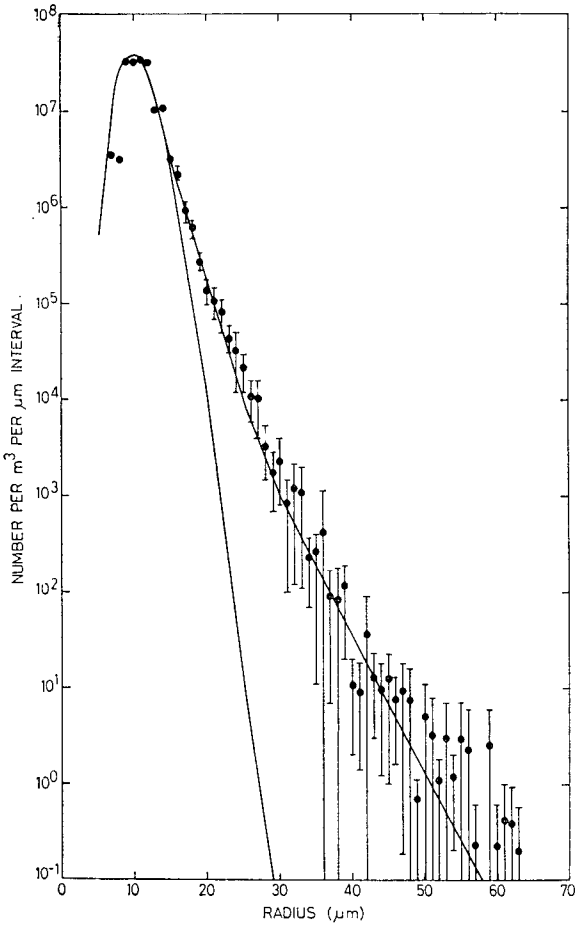

FIG. 3. The initial gamma distribution having 2×10^8 drops m^{-3} and the numerical solution to the coalescence equation after 900 s for the Klett and Davis collection kernels. The closed circles show the results from the Lapidus-Shafrir model and the error bars indicate the approximate 95% confidence intervals.

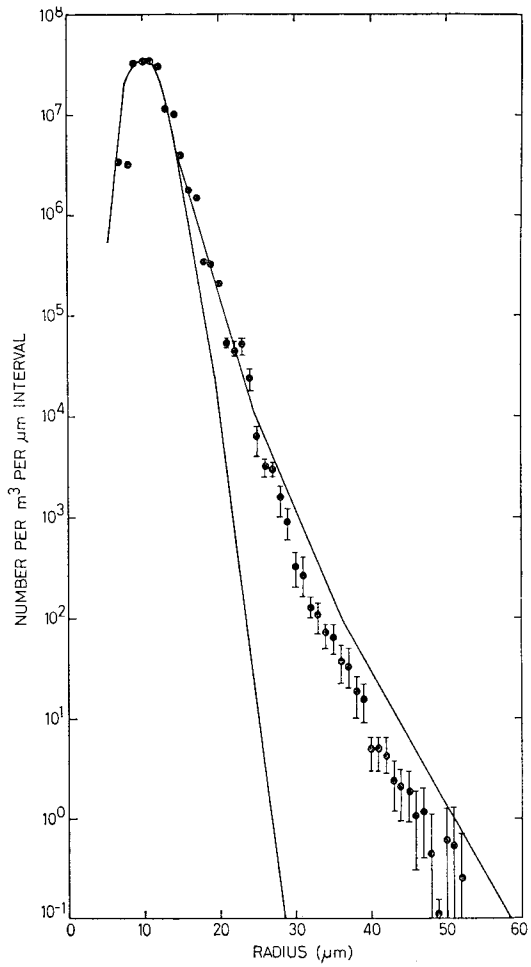

FIG. 4. As in Fig. 3 except that the closed circles show the results from the modified Lapidus-Shafrir model.

The Monte-Carlo procedures described above require that we sample randomly from a binomial distribution with parameters, say, n and K_{ij}. (In the Lapidus and Shafrir model $n=n_j$; in our modification $n=n_in_j$.) To do so, we have employed three different random variable generation techniques. For n less than 100 we use a uniform random number generator to conduct a "coin-tossing" process to generate the required random variable. When n is greater than 100 and nK_{ij} less than 25, the binomial distribution is approximated by a Poisson distribution with parameter nK_{ij}. A sample from the Poisson distribution is generated by a method given by Knuth (1969, p. 117). For nK_{ij} greater than 25 the Poisson distribution is approximated by a normal distribution with mean and variance nK_{ij}. Random normal deviates are generated by the Box-Muller-Knuth method (see Knuth, p. 105). (A secondary advantage of the modification proposed above is that the computationally simpler normal approximation is appropriate

in a much greater proportion of sampling occasions than it is in the original Lapidus and Shafrir model.)

A Monte-Carlo model more realistic than either the Lapidus and Shafrir model or the modified Lapidus and Shafrir model can be designed by sampling the number of n_j drop collected by *each* n_i drop. However, this procedure is computationally impracticable and therefore it is necessary to examine the validity of less exact models if a Monte-Carlo technique is to be used.

In the following section we compare the results of computations using a Lapidus and Shafrir model and a modified Lapidus and Shafrir model, and compare both sets of results with calculations made using the standard integral formulation of the coalescence process.

3. Comparative calculations

a. Golovin collection kernel

Calculations have been made using a collection kernel of the form described by Golovin (1963), i.e.,

$$K(x_i,x_j)=B(x_i+x_j),$$

where x_i and x_j are the masses of the collector and collected drops, respectively, and B is a constant. In these calculations B was 1.53×10^3 m^3 s^{-1} g^{-1}. The initial distribution is exponential in form, given by

$$n(x,t_0)=(N_0/x_0)\exp(-x/x_0),$$

where $n(x,t_0)$ is the number of drops m^{-3} g^{-1} at the initial time t_0, N_0 is 2.39×10^8 drops m^{-3}, and x_0 is 4.4×10^{-4} g. The temporal variation of this distribution, with the Golovin collection kernel, is known (see, e.g., Golovin, 1963; Scott, 1968). Figs. 1 and 2 both show this initial distribution, and the distribution after 400 s have elapsed. Also shown on both of these figures (and indicated by open circles) is the solution obtained from a numerical solution of the collection equation. The details of this numerical method are given by Ryan (1974), and it is seen that it provides a solution which agrees well with the analytical solution.

Fig. 1 shows the changes in the distribution after 400 s, as predicted by the Lapidus and Shafrir model. Each point plotted is the mean of a sample of 500 predictions of the number of drops of that radius. The standard error of the mean is also calculated from the sample, and used to calculate an approximate 95% confidence interval for the number of drops. This interval is indicated by the vertical bar through each point. Fig. 2 shows the changes, and associated confidence intervals, after 400 s, as predicted by the modified Lapidus and Shafrir model. Both Monte-Carlo models considerably underestimate the development of the tail of the distribution.

b. Klett and Davis collection kernels

The Klett and Davis (1973) collection kernels represent the most realistic collection kernels reported to date. We have used these in conjunction with two initial gamma distributions, each having a liquid water content of 1 g m^{-3} and a dispersion of 0.2. The first distribution has 2×10^8 drops m^{-3} while the second has 5×10^7 drops m^{-3}.

Fig. 3 shows the initial gamma distribution having 2×10^8 drops m^{-3} and the development of the distribution after 900 s as predicted by the numerical solution of the coalescence equations. Also shown are the results of applying the Lapidus and Shafrir model, together with the associated 95% confidence intervals. The Lapidus and Shafrir model suggests a more rapid development of the tail of the distribution than is indicated by the numerical solution. By contrast, Fig. 4, showing the results from the modified Lapidus and Shafrir model, suggests that this model slightly underestimates the development of the tail (at the 1 m^{-3} level by a factor of about 2).

Figs. 5 and 6 show the initial gamma distribution having 5×10^7 drops m^{-3}, and the development of the distribution after 900 s as predicted by the numerical solution of the coalescence equations. Fig. 5 shows the equivalent results from the Lapidus and Shafrir model and Fig. 6 those from the modified Lapidus and Shafrir model. As with the previous initial distribution, there is some evidence to suggest that the Lapidus and Shafrir model overestimates the development of the tail of the distribution. Fig. 6 shows that the modified Lapidus and Shafrir model underestimates the number of drops of large radius, at the 1 m^{-3} level, by a factor of about 5.

It should be noted that in Figs. 5 and 6 there is a change of scale, and of the number of Monte-Carlo samples averaged, at a radius of 100 μm. Particles of radius <100 μm are sorted into intervals 1 μm wide and those of radius >100 μm into intervals 10 μm wide. As a result, estimates for radii <100 μm are averages of 500 samples while those for radii >100 μm are averages of 5000 samples and hence have narrower confidence intervals.

4. Discussion

Calculations using the Golovin kernel and the exponential distribution indicate that the numerical solutions to the coalescence equations accurately model the change in the distribution with time, to concentrations less than 1 m^{-3}. It has also been pointed out elsewhere (see Ryan, 1974) that when the Klett and Davis collection kernels are used these calculations are in good agreement with similar calculations using the numerical techniques of Reinhart (1972). It will therefore be assumed that the numerical solutions of the coalescence equation as described by Ryan are a satisfactory standard against which to assess the Lapidus and Shafrir and the modified Lapidus and Shafrir models.

Figs. 1 and 2 show that both these models seriously underestimate the tail of the distribution. These find-

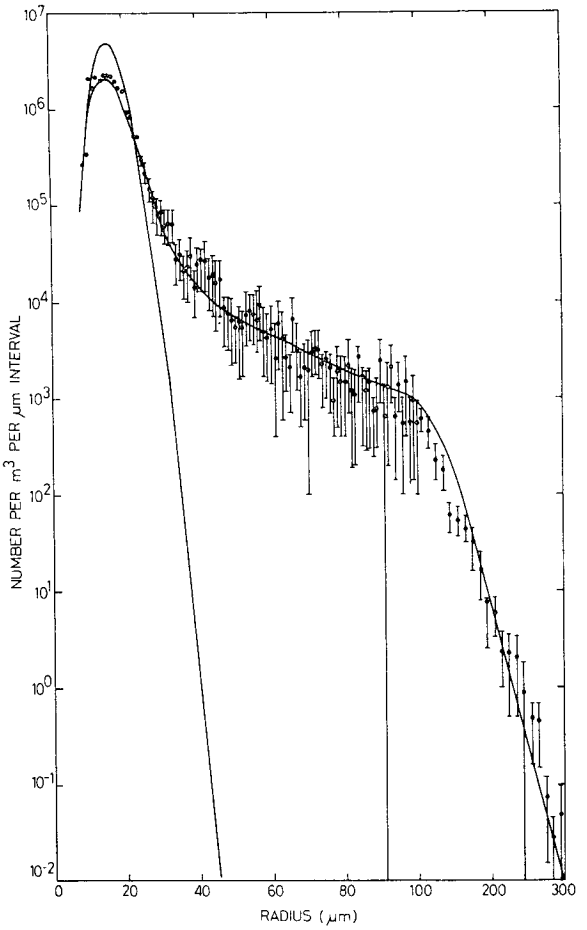

FIG. 5. The initial gamma distribution having 5×10^7 drops m^{-3} and the numerical solution to the coalescence equation after 900 s for the Klett and Davis collection kernels. The closed circles show the results from the Lapidus-Shafrir model and the error bars indicate the approximate 95% confidence intervals.

ings agree, in the case of the original model, with those reported by Lapidus and Shafrir (1972). The discrepancy between the modified Lapidus and Shafrir model and the analytical solution is readily accounted for by recognizing that the large Golovin collection kernel produces a relatively high number of occasions on which a drop collects many drops. As the radii of all the collector drops are assumed to grow at the same rate, the large drops resulting from these multiple collections are suppressed. The underestimation of the rate of production of large drops shown by the original Lapidus and Shafrir model is more difficult to explain, particularly as it has been pointed out that the model should overestimate the number of "rare" events. However, when we examine closely the computational course of the simulation, we find that for 500 experiments over 400 s there have been of the order of 800 "resets" initiated by "step 5" of the numerical procedure. That is, a very great number of "rare" events have been suppressed. (It should also be noted that the confidence intervals associated with the Lapidus and Shafrir model are much greater than those associated with the modified Lapidus and Shafrir model.) These numerical experiments suggest that both of the Monte-Carlo models are unsatisfactory when a relatively large collection kernel, such as the Golovin kernel, is used to describe coalescence.

The numerical experiments using the two gamma distributions and the Klett and Davis collection kernels yield a somewhat different conclusion. With both of the initial distributions the modified Lapidus and Shafrir model leads to only slight underestimation of the rate of development of large drops. At droplet concentrations of 1 m^{-3} the underestimation is by a factor of somewhere between 2 and 5.

By contrast, the Lapidus and Shafrir model tends to overestimate the rate of production of large drops. It is important to note that, with more realistic collection kernels, the initial distribution having 2×10^8 drops m^{-3} has only 14 "resets" by "step 5" for 500 experiments, while the initial distribution having 5×10^7 drops m^{-3} has 160 "resets" by "step 5." The confidence intervals associated with the Lapidus and Shafrir model

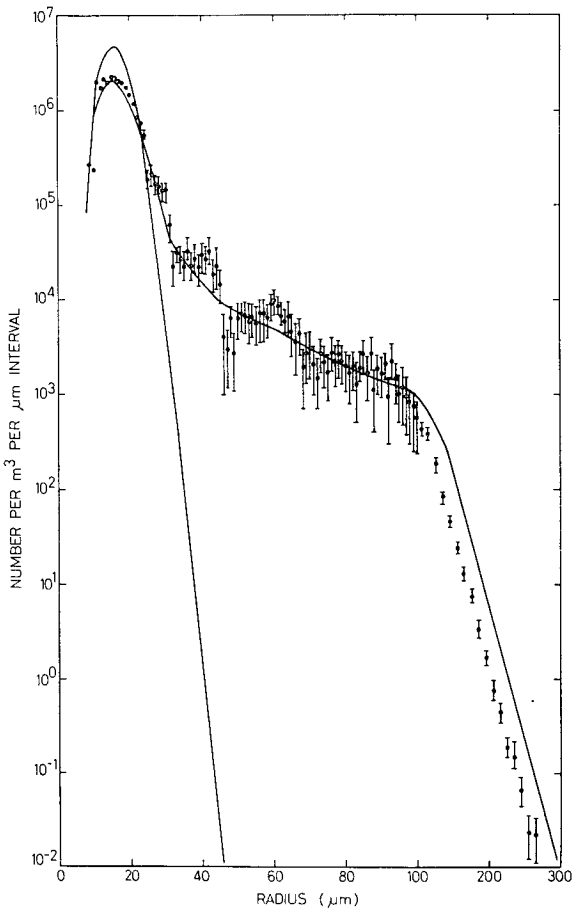

FIG. 6. As in Fig. 5 except that the closed circles show the results from the modified Lapidus-Shafrir model.

estimates are again much greater than those associated with estimates from the modified Lapidus and Shafrir model.

The oscillatory pattern in the tail of the distribution shown in Figs. 5 and 6 is spurious; it is a consequence of approximating a continuous density by a histogram.

It would appear from these results that the Monte-Carlo models do not lead to intolerable errors for times of the order of 1000 s when realistic collection kernels are used. However, it would appear that the modified Lapidus and Shafrir model is statistically sounder and that the procedure employed in "step 5" of suppressing "rare" events should only very occasionally occur.

There seems little point in using such an inexact method to describe the coalescence process when the integral equations are able to produce a solution from which the abovementioned inherent errors are absent. However, there are severe problems in modelling condensation and coalescence together. It is in this application that the Monte-Carlo model, when used with care, has proved to be very useful. The results of such simulations will be presented elsewhere.

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