Journal of Computational Physics **171,** 418–422 (2001)
doi:10.1006/jcph.2001.6776, available online at http://www.idealibrary.com on IDEAL®

NOTE

A New Formulation of the Spectral Multi-moment Method for Calculating the Kinetic Collection Equation: More Accuracy with Fewer Bins

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Received June 13, 2000; revised March 7, 2001

Key Words: kinetic collection equation; numerical solutions of integro differential equations.

1. INTRODUCTION

The numerical method used in solving the kinetic collection equation (KCE) considerably influences the accuracy of numerical simulations (e.g., cloud and precipitation development, coagulation of aerosol particles, etc.). In a former publication [6] (hereafter referred to as TRL) it was shown that the numerical solution obtained for the KCE by the spectral multi-moment method (SMMM) with a very high spectral resolution (144 spectral bins) approaches an exact solution of the KCE. It was suggested that this solution could be used as a reference for evaluating the accuracy of other numerical methods used for solving the KCE. Although the method is very useful as a reference solution to evaluate the performance of different numerical methods, it has the disadvantage that it requires a large number of spectral bins (144), making it impractical for use in models that include other dynamical or microphysical processes.

The existence of a reference solution stimulated the development of a relatively accurate and economical numerical method of solving the KCE. In the present work some modifications in the formulation of the SMMM are presented to permit the calculation of accurate results while maintaining a small number of bins, thus making the method more efficient. The new method is applied to 36 spectral bins and the results are compared with those

0021-9991/01 $35.00

obtained with the original algorithm using 36 and 72 bins and with the "reference" solution obtained with 144 bins.

2. METHOD DESCRIPTION

In TRL a detailed descripition of the solution of the KCE (Smoluchowski's equation) using the SMMM was presented. In this method the first two moments of the mass distribution function are solved at each spectral bin. The new algorithm differs from the original one by the use of (a) a different approach to formulating the approximation of the distribution function in the spectral bins and (b) a more accurate relationship between spectral moments in a bin.

(a) Equation (3) in TRL was used for approximating moments of the distribution function of the type $m^J f_k(m,t)$ (for $J = 0, 1, 2$) when integrals over incomplete bins appeared. That equation is replaced by

$$m^J f_k(m,t) = \frac{m_k^J}{(p-1)}\Psi_{J,k}(t)\left(p - \frac{m}{m_k}\right) + \frac{m_{k+1}^J}{(p-1)}\Phi_{J,k}(t)\left(\frac{m}{m_k} - 1\right). \tag{1}$$

In TRL the approximations were always based only on the first two moments (namely, $J = 0, 1$) and the functions $\Psi_{J,k}(t)$ and $\Phi_{J,k}(t)$ were the same for any J. In contrast, in the present new algorithm the two moments used in the approximation are not always the same but the selection depends on the moment one wants to evaluate; the subscript J in Ψ and Φ represents the moment that is being approximated. Following this approach, the approximation of $f_k(m,t)$ is done using the moments $J = 0$ and $1/2$, $m f_k(m,t)$ uses the moments $J = 1/2$ and 1 and $m^2 f_k(m,t)$ the moments $J = 1$ and 2.

$\Psi_{J,k}(t)$ and $\Phi_{J,k}(t)$ are found to be,

$$\text{for } J = 0 \begin{cases} \Psi_{0,k}(t) = \frac{2N_k(t)}{(p^{1/2}-1)(p-1)m_k}\left[p^{1/2} - \frac{S_k(t)}{m_k^{1/2}N_k(t)}\right] \\ \Phi_{0,k}(t) = \frac{2N_k(t)}{(p^{1/2}-1(p-1)m_k}\left[\frac{S_k(t)}{m_k^{1/2}N_k(t)} - 1\right] \end{cases}, \tag{2}$$

$$\text{for } J = 1 \begin{cases} \Psi_{1,k}(t) = \frac{2N_k(t)}{(p^{1/2}-1)(p-1)m_k}\left[p^{1/2}\frac{S_k(t)}{m_k^{1/2}N_k(t)} - \frac{M_k(t)}{m_kN_k(t)}\right] \\ \Phi_{1,k}(t) = \frac{2N_k(t)}{p^{1/2}(p^{1/2}-1)(p-1)m_k}\left[\frac{M_k(t)}{m_kN_k(t)} - \frac{S_k(t)}{m_k^{1/2}N_k(t)}\right] \end{cases}, \tag{3}$$

and

$$\text{for } J = 2 \begin{cases} \Psi_{2,k}(t) = \frac{2N_k(t)}{(p-1)^2m_k}\left[p\frac{M_k(t)}{m_kN_k(t)} - \frac{Z_k(t)}{m_k^2N_k(t)}\right] \\ \Phi_{2,k}(t) = \frac{2N_k(t)}{p(p-1)^2m_k}\left[\frac{Z_k(t)}{m_k^2N_k(t)} - \frac{M_k(t)}{m_kN_k(t)}\right] \end{cases}, \tag{4}$$

where $N_k(t)$, $M_k(t)$, and $S_k(t)$ represent the moments 0, 1, and $1/2$, respectively.

The formulation of the approximation in Eq. (1) is independent of the kernel of interaction or the physical problem. The approximation must fulfill three physical requirements: (a) the function must be positive within the bin interval, (b) the total mass of the distribution must be conserved (moment $J = 1$), and (c) a balance between the mass concentration and the number concentration (moment $J = 0$) in each bin should be maintained; namely, the average mass should remain between the bin boundaries.

(b) In [4] and in TRL a nondimensional parameter ξ that relates three neighboring moments was introduced in order to close the equations (Eq. (6) in TRL). The range of variation of ξ is between 1 and 17/16, namely 6.25%. Therefore, in the calculation of the higher moments ξ introduces an inaccuracy that varies between 6.25% for the second moment ($Z_k(t)$) and 44% for the fourth moment ($M_k^{(4)}(t)$).

In order to reduce these inaccuracies, higher moments are calculated using a modified expression for ξ,

$$M_k^J(t) = \xi_{J,p}\left[\frac{M_k(t)}{N_k(t)}\right]^{J-1} M_k(t), \tag{5}$$

where the nondimensional parameter ξ is also determined by the desired moment.

The expressions for $\bar{\xi}$ for $J = 1/2, 2, 3, 4$ and $p = 2$ can be formulated as

$$\begin{aligned}
\bar{\xi}_{1/2} &= 0.25\left\{2 + \left[\frac{m_k N_k(t)}{M_k(t)}\right]^{-0.5} + \left[\frac{m_k N_k(t)}{M_k(t)}\right]^{0.5}\right\}\\
\bar{\xi}_2 &= 0.5\left\{1 + 3\left[\frac{m_k N_k(t)}{M_k(t)}\right] - 2\left[\frac{m_k N_k(t)}{M_k(t)}\right]^2\right\}\\
\bar{\xi}_3 &= 0.5\left\{1 + 2\left[\frac{m_k N_k(t)}{M_k(t)}\right] + \left[\frac{m_k N_k(t)}{M_k(t)}\right]^2 - 2\left[\frac{m_k N_k(t)}{M_k(t)}\right]^3\right\}\\
\bar{\xi}_4 &= 0.25\left\{2 + 5\left[\frac{m_k N_k(t)}{M_k(t)}\right] + \left[\frac{m_k N_k(t)}{M_k(t)}\right]^2 - 8\left[\frac{m_k N_k(t)}{M_k(t)}\right]^3 + 4\left[\frac{m_k N_k(t)}{M_k(t)}\right]^4\right\}.
\end{aligned} \tag{6}$$

These expressions significantly reduce the inaccuracies in ξ. For example, for the fourth moment the inaccuracy is now only 5.2%, compared to 44% using the former formulation.

3. RESULTS

Numerical simulations of cloud drop growth by collection were conducted for three different kernels: Golovin [1], for which an analytic solution exists, and the hydrodynamical kernel with collection efficiencies by Hall [2] and Long [3]. The initial cloud drop mass distribution function was represented by an exponential function with a total number concentration of 300 particles cm^{-3} and a total mass of 1, 2, and 3 g m^{-3}. In all cases the minimum radius r_1 was 1.5625 μm and the maximum $r_{\max}$ was 6400 μm. Simulations with the new algorithm were conducted for $p = 2$ (36 bins). In all numerical experiments, total mass was conserved.

Results for Golovin's kernel with a total mass of 1 g m^{-3} show that up to 0.65 mm the numerical results obtained with the new algorithm are similar to the analytical solution. For larger diameters the new results are still better than those obtained with 108 bins and very close to those obtained with 144 bins. Numerical simulations were also conducted for two hydrodynamical kernels for which no analytical solutions exist. The new formulation was evaluated for Long's and Hall's kernels for a total mass concentration of 1, 2, and 3 g m^{-3}. As an example, results obtained for Long's and Hall's kernels for 2 g m^{-3} after 10 min of simulation are shown in Figs. 1a and 1b, respectively. In all these cases, the results are

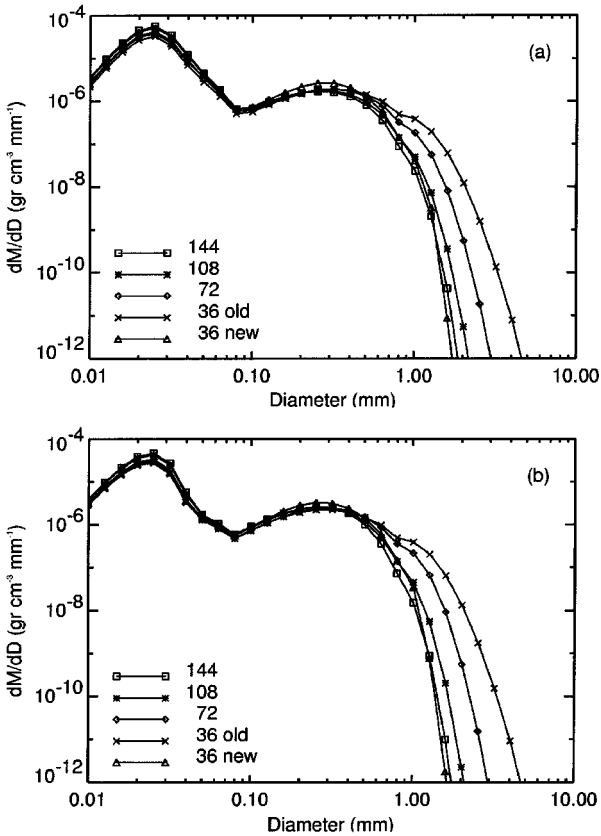

FIG. 1. Mass concentration distribution for (a) Long's and (b) Hall's hydrodynamical kernels after 10 min of simulation. The total mass concentration is 2 g m^{-3}.

compared with those obtained with 144 bins, considered as "reference." For both kernels the numerical results with the new algorithm are significantly closer to the reference than the original one. The results are even better than those obtained with 108 bins.

In order to quantitatively evaluate the accuracy of the results obtained with the different formulations the mass concentration accumulated in 14 bins (containing 99.9% of the total mass) was evaluated. The 14 bins correspond to those defined by the 36 bins division. The evaluation consisted of calculating the average and standard deviation of the ratios between the mass at one of the 14 bins from one of the formulations and the mass predicted by the "reference" solution. Namely,

$$\frac{1}{14}\sum_{k=k^*}^{k^*+14}\frac{M_k^{(\#)}}{M_k^{(144)}}, \tag{7}$$

where $M_k^{(\#)}$ represents the mass at bin k from one of the formulations (36 bins new, 72, or 108). The evaluation was conducted for the numerical experiment using Long's kernel, a total mass concentration of 2 g m^{-3}, and after 20 min of simulation. The results thus calculated show that the new formulation with 36 bins differed from the reference solution (144 bins) by 4.5% with a standard deviation of 3.2%. The new formulation was even more accurate than the 108 bins model which differed from the reference solution by

10.8% on the average with a standard deviation of 8.3%. According to these results one can claim that the new formulation performs similarly to the 108 bins model but required significantly less computation time, by a factor of 25. When compared to the 72 bins case the new method is much more accurate and requires about five times less computation time.

4. CONCLUSIONS

A new formulation of the approximation of the distribution function used in the spectral multi-moments method was developed and implemented in the numerical solution of the kinetic collection equation. In the new approximation there is a correspondence between the moment one wants to evaluate and the moments used in the approximation. This new method provides an accurate and efficient numerical solution of the KCE, appropriate for use in dynamical cloud models. The results show a significant improvement in the accuracy of the calculations while maintaining a low number of bins and high computation efficiency, independent of the initial distribution and kernel used. Compared to the original SMMM the computation time in the present method can be reduced by more than one order of magnitude while maintaining similar accuracy.

ACKNOWLEDGMENTS

Special thanks are due to Mrs. Zipi Rosen and Mrs. Sara Rehavi for their help with the programming and the testing of the code, without which this work would have never been accomplished. Part of this work was conducted under a grant from the German–Israeli Foundation (GIF) under Contract I-544-156.08/97.

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