

# Evolution of Discrete Coagulation Equation

HAMID R. KOBRAEI<sup>1</sup> AND G. COMER DUNCAN

*Department of Physics and Astronomy, Bowling Green State University, Bowling Green, Ohio 43403-0224*

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A new approximation technique is suggested for coagulation equations which is remarkably accurate. This technique leads to a new form for the discrete coagulation equation. This method has been applied to several different initial distributions for both physical and mathematical kernels. Furthermore, our method indicates that taking the first moment as a criterion for accuracy of the integration method is misleading and yields erroneous conclusions. The approximate polynomial solution to the coagulation equations for an arbitrary kernel has also been investigated. It is found that the polynomial solution is very accurate and easy to apply for the case of a constant kernel but, for a variable kernel, it may be applied only to cases where the fluctuation of the kernel from its average value is very small. The appearance of the second peak for the initial gamma distribution is observed for all kernels applied here.

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## I. INTRODUCTION

In the theory of the coagulation of aerosol particles one assumes that the rate of change of the number of particles of size  $k$ ,  $n(k, t)$  (volume  $v_k = kv_{\text{basic}}$ ), in the discrete case is given by

$$\frac{dn(k, t)}{dt} = \frac{1}{2} \sum_{j=1}^{k-1} \beta(k-j, j)n(k-j, t)n(j, t) - n(k, t) \sum_{i=1}^{\infty} \beta(k, i)n(i, t). \quad [1]$$

Different kernels  $\beta(i, j)$  are inserted, depending on the particular limit for those  $\beta(i, j)$ 's which represent physically well-motivated situations. Only the model  $\beta(i, j)$ 's for the cases where  $\beta(i, j) \propto \beta_0$ ,  $\beta(i, j) \propto i + j$ , and  $\beta(i, j) \propto ij$  have thus far yielded analytical solutions. Thus, in realistic situations one is led to the coagulation equations. There has been considerable work reported along these lines (1–5). However, these attempts have not resulted in evolutions of the size distribution which are

adequately stable in time and adequately accurate. There is a need in such evolutions to integrate the coagulation equations over a long time. The above two problems always seem to arise if the integration time is over several characteristic times.

It is with this need to have sufficiently accurate and stable long time evolutions that the present work arose. In the coagulation equation, Eq. [1], the depletion term involves the process by which a particle of size  $k$  can combine with any other size which is initially present to form a particle of size larger than  $k$ . In this process size  $k$  particles disappear. Note that the sum in Eq. [1] is in principle over *all* sizes. Assuming no upper limit for the size of a particle, the sum must go to infinite size. However, in any computer implementation of the coagulation equations only a *finitely* large number of particles may be included. One essentially implicit operating assumption in previous direct numerical integrations of the coagulation equations has been that one may get accurate long term solutions by making the maximum particle size,  $n_{\text{max}}$ , of the order of a few hundred. Of course, the aim of evolutions is to follow the long-time behavior of  $n(k, t)$  for  $k = 1, \dots, n_{\text{max}}$ . It seems to have

<sup>1</sup> Current address: Center for Aerosol Research, Physics & Astronomy, Murray State University, Murray, KY 42071.

been the case that previous investigators have limited the maximum size number but still have not achieved the desired goal of accurately integrating for many characteristic times (6, 7). We contend here that the goal of accurate, stable, long-term evolution with a *finite* maximum size number is doomed to failure. Whenever one truncates the sum in the second term of Eq. [1] there will develop a nontrivial error which will propagate and, long before the long time evolution is finished, severely impact the results. Such phenomena were mentioned by Gelbard and Seinfeld (10b). This problem has been referred to as the finite domain problem (10b).

Given that one can not include an infinite number of particle sizes on a finite-memory computer, what recourse is there? A clue as to a way around this impasse can be seen from a consideration of the behavior of the physical  $\beta(i, j)$ 's. In the theory of the Brownian motion of aerosol particles, there are essentially three types of physically well-motivated  $\beta(i, j)$ 's: Those of the free molecular regime ( $kn > 10$ ), those of the continuum regime ( $kn < 0.1$ ), and those of the transitional regime ( $0.1 \leq kn \leq 10$ ) (8, 12, 15, 16). In Figs. 1 and 2 we show plots of the  $\beta(i, j)$ 's for the free molecular and continuous regimes as functions of  $i$  and  $j$ . One sees immediately from these surfaces that the physical  $\beta(i, j)$ 's have a large region in the  $(i, j)$  plane where they are quite slowly varying. It is only very near the  $i = 1, j = 1, \dots$  and the  $j = 1, i = 1, \dots$  rows that there is significant variation. The point of this observation

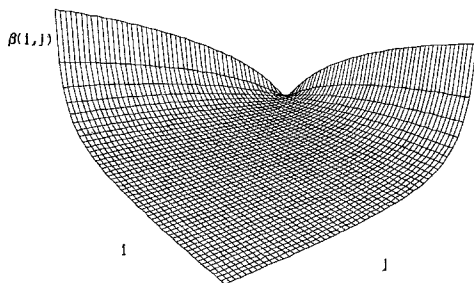


FIG. 1. The free molecular regime kernel  $\beta(i, j) = \beta_0 \times (j/i + i/j)^{1/2}(i^{1/3} + j^{1/3})^2$  is plotted as a function of  $i$  and  $j$ .

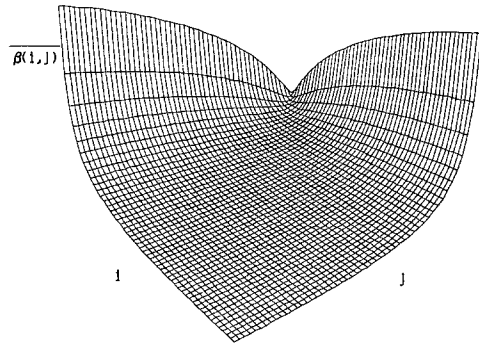


FIG. 2. The continuum regime kernel  $\beta(i, j) = \beta_0 \times (i^{1/3} + j^{1/3})(i^{-1/3} + j^{-1/3})$  is plotted as a function of  $i$  and  $j$ .

is that for larger and larger values of  $i$  and  $j$ , other than the "edges," the  $\beta(i, j)$ 's are reasonably well approximated by the constant case. Since this approximately constant  $\beta(i, j)$  behavior becomes better and better the larger the maximum values of  $i$  and  $j$ , it might be useful to consider the constant  $\beta(i, j)$  behavior in relating the contribution of the part of the sum from  $n_{\max}$  to infinity to the rate at which particles of size  $k$  are depleted. It is the focus on this asymptotic behavior which leads us to a new approximation method.

Here we give two methods for dealing with the problems associated with keeping only a finite number of terms in the second sum. Let us define the following useful variables:

$$Z(k, t) = n(k, t)/N_0, \quad [2]$$

where  $N_0$  is the total number of particles of all sizes present at  $t = 0$ ;

$$N_0 = \sum_{i=1}^{\infty} n(i, 0). \quad [3]$$

Second, let

$$K(i, j) = \beta(i, j)/\langle \beta \rangle, \quad [4]$$

where

$$\langle \beta \rangle = \frac{1}{N^2} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} n(i, t)n(j, t)\beta(i, j) \quad [5]$$

and

$$N(t) = \sum_{i=1}^{\infty} n(i, t). \quad [6]$$

## II. POLYNOMIAL SOLUTION

Consider the depletion term in Eq. [1]. Now we see in Figs. 1 and 2 that there is a large region in  $(i, j)$  space where  $\beta(i, j)$  is quite slowly varying. This leads us, as a first approximation, to replace the last term by (11)

$$-n(k, t) \sum_{i=1}^{\infty} \beta(k, i) n(i, t) \approx -n(k, t) \langle \beta \rangle N(t) \quad [7]$$

where the time dependent quantities  $\langle \beta \rangle$  and  $N(t)$  have been defined above in Eqs. [5] and [6]. This yields the approximate coagulation equations

$$\frac{dn(k, t)}{dt} = \frac{1}{2} \sum_{j=1}^{k-1} \beta(k-j, j) n(k-j, t) n(j, t) - n(k, t) \langle \beta \rangle N(t). \quad [8]$$

We now demonstrate that there exists a class of polynomial solutions to Eq. [8] (9–11). First we reexpress Eq. [8] in terms of the  $Z(k, t)$  defined in Eq. [2]. We have

$$\frac{2}{N_0 \langle \beta \rangle} \frac{dZ(k, t)}{dt} = \sum_{j=1}^{k-1} K(k-j, j) \times Z(k-j, t) Z(j, t) - 2Z(k, t) N(t)/N_0. \quad [9]$$

However, the time derivative of the total number of particles may be found by summing Eq. [1] over all particle sizes:

$$\frac{dN(t)}{dt} = -\frac{1}{2} \langle \beta(t) \rangle N^2.$$

Then,

$$N(t) = N_0 / \left[ 1 + \int_0^t \frac{N_0 \langle \beta(t') \rangle}{2} dt' \right]. \quad [10]$$

We make a change of time variable to

$$T = 1 + \int_0^t \frac{N_0 \langle \beta(t') \rangle}{2} dt'. \quad [11]$$

The relation [9] in terms of a new time variable and with the aid of Eq. [10] takes the form

$$\frac{dZ(k, T)}{dT} = \sum_{j=1}^{k-1} K(k-j, j) Z(k-j, T) Z(j, T) - \frac{2Z(k, T)}{T}. \quad [12]$$

The polynomial solution is most naturally expressed in terms of the variable

$$\lambda = 1 - 1/T. \quad [13]$$

Introducing Eq. [13] into Eq. [12] yields

$$\frac{d(T^2 Z(k, T))}{d\lambda} = \sum_{j=1}^{k-1} K(k-j, j) \times (T^2 Z(k-j, T)) (T^2 Z(j, T)).$$

If we write  $Z(k, T)$  as a polynomial in  $\lambda$

$$Z(k, T) = \frac{1}{T^2} \sum_{\alpha=1}^k B_{k,\alpha} \lambda^{\alpha-1} \quad [14]$$

we find that Eq. [12] is satisfied if the  $B_{k,\alpha}$  obeys

$$B_{k,\alpha} = \frac{1}{(\alpha-1)} \sum_{j=1}^{k-1} K(k-j, j) \sum_{\beta+\gamma=\alpha} B_{k-j,\beta} B_{j,\gamma} \quad \text{for } \alpha \geq 2. \quad [15]$$

Here  $B_{k,1} = C_k \equiv Z(k, 1)$ . This is a recursive definition for  $B_{k,\alpha}$ . The polynomial solution is valid for an arbitrary kernel and an arbitrary initial distribution subject, of course, to the approximation Eq. [7]. Unlike other polynomial solutions (11) the polynomial solution (9) in Eq. [14] has the advantage of keeping the kernel in its natural form and uses  $T$  as the time variable (2, 4, 14) rather than real time.

The polynomial solution may be efficiently generated once the kernel  $\beta(i, j)$  and the initial distribution  $Z(k, 1)$  are given. Now in the special case of a constant kernel the polynomial solutions described above become the exact solution to the coagulation equation (Eq. [1]).

We have applied the polynomial solution to several kernels and compared the results to the analytical and the direct numerical integration of the coagulation equation. To explore the properties of the polynomial solution for a constant kernel, we consider the normalized initial gamma distributions given by

$$C(x) = Z(x, 1) = \frac{P^P x^{P-1} e^{-Px}}{(P-1)!} \quad P = 1, 2, \dots \quad [16]$$

where  $C(x)$  is the concentration of particles of volume  $x$  at  $t = 0$ . Analytical solution of the initial gamma distributions is well known. For  $P = 2$ , the analytical solution for the distribution in Eq. [16] has the form

$$Z(x, T) = \frac{1}{T^2} \frac{2e^{-2x}}{\sqrt{\lambda}} \sinh(2x\sqrt{\lambda}) \quad [17]$$

where  $Z(x, T)$  gives the concentration of particles at any given time and  $\lambda$  is given by Eq. [13].

On the other hand, the polynomial solution, Eq. [14], with a constant kernel takes the recursive form

$$Z(k, T) = \frac{C(k)}{T^2} + \lambda \sum_{j=1}^{k-1} C_{(k-j)} Z(j, T). \quad [18]$$

We have compared the results of the polynomial solution, Eq. [18], with the analytical solution, Eq. [17], for the initial gamma distribution with  $P = 2$ . The agreement between the two methods is remarkably close. The evolution of the initial gamma distribution with  $p = 2$  from the polynomial method given in Eq. [18] is given in Fig. 3.

The polynomial solution, Eq. [18], has also been applied to narrow distributions. For the sufficiently narrow distributions, the appearance of a second peak in the evolution of the size distribution is observed. Results of both the analytical and the direct numerical integration of the coagulation equation have con-

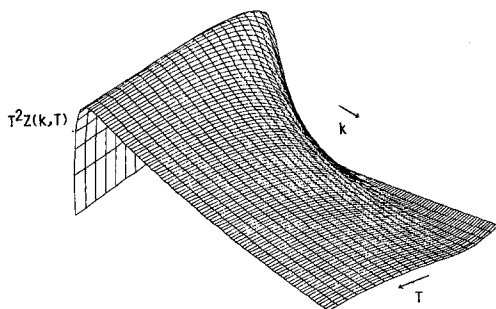


FIG. 3. The evolution of the initial gamma distribution with  $P = 2$  for the case of a constant kernel from the polynomial method given in [16]. Here the evolution is plotted up to  $T = 11$ .

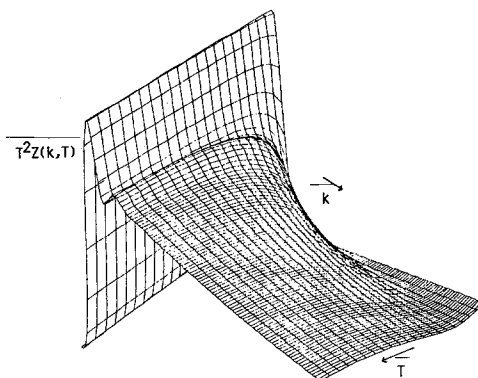


FIG. 4. The evolution of the initial gamma distribution with  $P = 9$  for the case of a constant kernel from the polynomial solution given in [16]. Here the evolution is plotted up to  $T = 11$ .

firmed this phenomenon. We have applied the polynomial solution to the family of initial gamma distributions, Eq. [16], with  $P = 1, 2, \dots, 9$ . In doing this the second peak is observed around  $P = 5$ . In Fig. 4, the evolution of initial gamma distribution with  $P = 9$  is given.

As long as the fluctuation of the variable kernel is small relative to its average, Eq. [5], the polynomial solution continues to provide results which are adequately accurate. The continuum regime kernel

$$\beta(i, j) = \beta_0(i^{-1/3} + j^{-1/3})(i^{1/3} + j^{1/3}), \quad [19]$$

where  $\beta_0$  is constant, has negligible fluctuation from its average value, as can be seen in Fig. 2. For example in Figs. 5 and 6, the numerical integration and the polynomial solution of the initial gamma distribution with  $P = 2$  are given, using the continuum and the free molecular regime kernels, respectively.

However, for kernels with noticeable fluctuation from their average values, for instance,

$$\beta(i, j) = \beta_0(i + j), \quad [20]$$

the polynomial solution will no longer provide reasonable results. Evidence of this discrepancy can be seen by referring to Fig. 7, where the polynomial solution, Eq. [14], is applied. Therefore, one has to seek other alternatives.

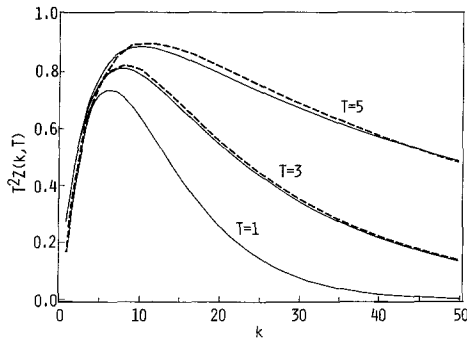


FIG. 5. The evolution of the initial gamma distribution with  $P = 2$  using the continuum regime kernel from the polynomial solution, Eq. [14], and the new coagulation equation, Eq. [24] (solid lines).

One such alternative is introduced in the next section. The error analysis of the polynomial solution is given in Section IV.

### III. INFINITE TAIL APPROXIMATION

We also introduce another approximation to the coagulation equations which, as we shall show, is even more robust with respect to how it handles the finite domain problem.

Let us write the exact coagulation equation in terms of the  $Z(k, T)$  variables introduced above, but not making any approximations. We find

$$\frac{dZ(k, T)}{dT} = \sum_{j=1}^{k-1} K(k-j, j)Z(k-j, T)Z(j, T)$$

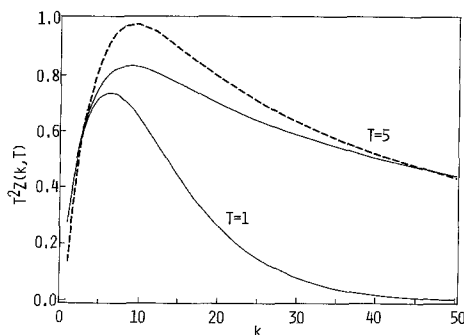


FIG. 6. The evolution of the initial gamma distribution with  $P = 2$  using the free molecular regime kernel from the polynomial solution, Eq. [14], and the new coagulation equation, Eq. [24] (solid lines).

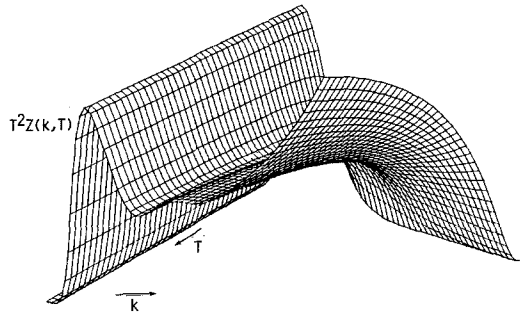


FIG. 7. The evolution of the initial gamma distribution with  $P = 9$  for the kernel  $\beta(i, j) = \beta_0(i + j)$  from the polynomial solution given in (12). Here the evolution is plotted up to  $T = 9$ .

$$\begin{aligned} & -2 \sum_{i=1}^{n_{\max}} K(i, k)Z(i, T)Z(k, T) \\ & -2 \sum_{i=n_{\max}+1}^{\infty} K(i, k)Z(i, T)Z(k, T). \quad [21] \end{aligned}$$

This is just another form of Eq. [1]. It is at this point that we make an approximation.

If one had a *constant*  $\beta(i, j) = \beta_0$ , then  $\langle \beta \rangle = \beta_0$  and  $K(i, k) = 1$  for all  $i$  and  $k$ . Also,  $N(t) = N_0/T$ . Now consider the sum

$$\begin{aligned} \frac{N}{N_0} &= \sum_{i=1}^{\infty} Z(i, T) \\ &= \sum_{i=1}^{n_{\max}} Z(i, T) + \sum_{i=n_{\max}+1}^{\infty} Z(i, T). \quad [22] \end{aligned}$$

Thus,

$$\sum_{i=n_{\max}+1}^{\infty} Z(i, T) = \frac{1}{T} - \sum_{i=1}^{n_{\max}} Z(i, T). \quad [23]$$

Assuming  $K(i, k) = 1$  for  $n_{\max} + 1 \leq i < \infty$  and with the help of Eq. [23], Eq. [21] takes the form

$$\begin{aligned} \frac{dZ(k, T)}{dT} &= \sum_{j=1}^{k-1} K(k-j, j)Z(k-j, T)Z(j, T) \\ & -2 \sum_{i=1}^{n_{\max}} K(i, k)Z(i, T)Z(k, T) \\ & -2Z(k, T) \left( \frac{1}{T} - \sum_{i=1}^{n_{\max}} Z(i, T) \right). \end{aligned}$$

Hence

$$\begin{aligned} \frac{dZ(k, T)}{dT} = & \sum_{j=1}^{k-1} K(k-j, j)Z(j, T)Z(k-j, T) \\ & - 2Z(k, T) \sum_{i=1}^{n_{\max}} [K(i, k) - 1]Z(i, T) - \frac{2Z(k, T)}{T}. \end{aligned} \quad [24]$$

Equation [24] constitutes the basic equations of the new approximation scheme. Note that we have (a) split off a  $T^{-1}$  time-dependent rate at which particles of size  $k$  disappear and (b) altered the relative  $K(i, k)$  to  $K(i, k) - 1$ . There are still a finite number,  $n_{\max}$  of sizes in any specific evolution. We will discuss the results of using Eq. [24] in place of Eq. [1] in applications. It turns out that this method yields results with much superior accuracy and apparent stability. In essence this method splits off the dominant contributions to the long time, large size behavior. This splitting isolates the important behavior and serves to control any deleterious feedback of the finite domain problem.

We have integrated the new coagulation, Eq. [24], for several kernels (physical as well as mathematical) with different initial size distributions. Let us first consider the case of a constant kernel. Here the result is the same as that obtained from both the polynomial solution, Eq. [18], and the analytical solution, Eq. [16].

We have also tested Eq. [24] for variable kernels. For an initial gamma distribution with  $P = 2$ , the results of Eq. [24] and the polynomial solution, Eq. [14], are given in Figs. 5 and 6 using the continuum and the free molecular regime kernels, respectively. The evolution of the initial gamma distribution with  $P = 9$  and  $P = 2$  are given in Figs. 8 and 9 for the continuum regime and the kernel given by Eq. [20], respectively. Comparison of our results with the direct numerical integration of Eq. [1] indicates the following. For up to 1000 in Eq. [1], one only needs to choose  $n_{\max}$  in the new coagulation equation, Eq. [24], equal to 100 to obtain essentially identical re-

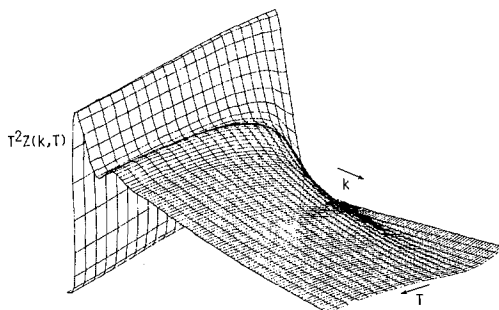


FIG. 8. The evolution of the initial gamma distribution with  $P = 2$  for the continuum regime kernel. Here the evolution is plotted up to  $T = 9$ .

sults. Furthermore, Eq. [24] does not suffer from the accumulation of error as the integration [1] does. The error analysis of the new coagulation equation method and the direct integration of [1] are discussed in the next section.

#### IV. ERROR ANALYSIS

In this section we discuss the error associated with the direct numerical integration of the coagulation equation, Eq. [1]. Then, the result of this analysis will be compared with the two other alternative methods, namely, the polynomial solution, Eq. [14], and the new approximate coagulation equation, Eq. [24].

A problem that arises with the numerical integration of the coagulation equation is that it yields an erroneous value for the particle concentration for sizes close to the truncation point  $n_{\max}$ . This results from truncating the depletion term in Eq. [1]. When the depletion term is truncated, in essence, a small contribution is made to the creation term leading to higher particle concentrations. This is depicted in Fig. 10 where the concentration of a particle of size 50 (volume =  $50V_0$ ) is shown as a function of time for values of  $n_{\max} = 50$  and  $n_{\max} = 200$ .

The error generated in each time step of the numerical integration of Eq. [1] is given by

$$\epsilon_j = \Delta T \left[ \frac{dZ(j, T)}{dT} - \frac{dZ_{tr}(j, T)}{dT} \right]$$

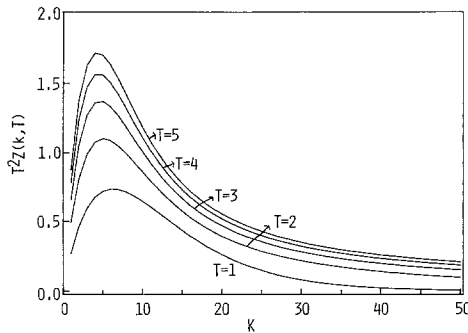


FIG. 9. The evolution of the initial gamma distribution with  $P = 2$  using the kernel  $\beta(i, j) = \beta_0(i + j)$  from the new coagulation equation, Eq. [24].

or

$$\begin{aligned} \epsilon_j = \Delta T \{ & \sum_{i=1}^{j-1} [Z(i, T)Z(j-i, T) \\ & - Z_{tr}(i, T)Z_{tr}(j-i, T)]K(j-i, i) \\ & - 2 \sum_{k=1}^{n_{\max}} [Z(j, T)Z(k, T) - Z_{tr}(j, T)Z_{tr}(k, T)] \\ & \times K(j, k) - 2 \sum_{k=n_{\max}+1}^{\infty} Z(k, T)Z(j, T)K(j, k) \} \end{aligned} \quad [25]$$

where the difference inside the brackets arises due to the truncation of the coagulation equation. Then, the error for all particle sizes in the distribution in each time step  $\Delta T$  may be written as

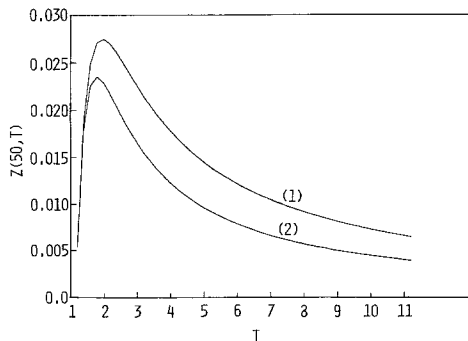


FIG. 10. The particle concentration of size 50 is plotted as function of  $T$  for (1)  $n_{\max} = 50$ , (2)  $n_{\max} = 200$ .

$$E = \sum_j \epsilon_j. \quad [26]$$

Even for the case constant kernel where

$$K(i, j) = 1 \quad \text{for } i = 1, 2, \dots, j = 1, 2, \dots$$

the numerical integration of Eq. [1] will lead to erroneous values of particle concentrations. This is due to the last term of Eq. [25] which is nonzero. The effect of truncating the depletion term on the behavior of smaller size particles is shown in Fig. 10, where the kernel of Eq. [20] is employed. The direct numerical integration of Eq. [1] even for the continuum regime kernel yields results which differ from those of Eq. [24] with the same value for  $n_{\max}$ . For particles of size 50 (volume =  $50V_0$ ), the results of both Eq. [1] and the new coagulation equation, Eq. [24], are given in Fig. 11. In this figure the continuum regime kernel is employed and  $n_{\max}$  is the same for both curves and equal to 100.

Similar to relations [25] and [26], the error associated with the polynomial solution [14] in a time step can be written in the form

$$\begin{aligned} \epsilon_j = \Delta T \{ & \sum_{i=1}^{j-1} [Z(i, T)Z(j-i, T) \\ & - Z_p(i, T)Z_p(j-i, T)]K(j-i, i) \\ & - 2 \sum_{i=1}^{\infty} [Z(i, T)Z(j, T)K(i, j) \\ & - Z_p(i, T)Z_p(j, T)] \}. \end{aligned} \quad [27]$$

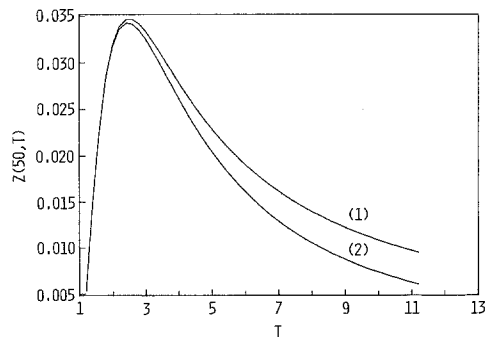


FIG. 11. The particle concentration of size 50 is plotted as function of  $T$  from (1) the direct integration of Eq. [1] and (2) the integration of Eq. [24].

As can be seen from the above relation, the polynomial solution has no theoretical error for the case of a constant kernel. Therefore, the polynomial solution can be used to study the long-time behavior of any initial distribution with a constant kernel. However, for a variable kernel the accuracy of the polynomial solution depends on the value of  $K(i, j)$ . The polynomial solution may be applied to the cases where the average fluctuation of normalized kernels is very small. One such case, as mentioned earlier, would be the continuum kernel, Fig. 5.

We contend that integrating the new coagulation equation, Eq. [24], serves as a better alternative to Eq. [1] for variable kernels as well as for constant kernels. Also, it is a good replacement to the polynomial solution for the case of variable kernels since the error associated with the new coagulation equation, Eq. [24], in each time step is given by

$$\begin{aligned} \epsilon_j = \Delta T \{ & \sum_{i=1}^{j-1} [Z(i, T)Z(j-i, T) - Z_n(i, T) \\ & \times Z_n(j-i, T)]K(j-i, i) - 2 \sum_{i=1}^{n_{\max}} [Z(i, T) \\ & \times Z(j, T) - Z_n(i, T)Z_n(j, T)]K(i, j) \\ & - 2 \sum_{i=n_{\max}+1}^{\infty} [Z(i, T)Z(j, T)K(i, j) \\ & - Z_n(i, T)Z_n(j, T)] \}. \quad [28] \end{aligned}$$

Unlike Eq. [25], no theoretical error is associated with the numerical integration of the new coagulation equation [24] for the case of a constant kernel. If one assumes  $Z(i, T) \approx Z_n(i, T)$  at time  $= T$ , then the error associated with the new coagulation equation, Eq. [28], becomes

$$\epsilon_j \approx -2 \sum_{i=n_{\max}+1}^{\infty} Z(i, T)Z(j, T)[K(i, j) - 1]\Delta T. \quad [29]$$

The error in each time step, Eq. [26], takes the form

$$E \approx -2 \sum_{j=1}^{\infty} \sum_{i=n_{\max}+1}^{\infty} Z(i, T)Z(j, T) \times [K(i, j) - 1]\Delta T. \quad [30]$$

With the help of Eq. [5] and finite  $n_{\max}$ , the theoretical error of Eq. [24] behaves like

$$E \rightarrow -2\Delta T \left( \frac{N^2}{N_0^2} - \frac{N^2}{N_0^2} \right). \quad [31]$$

Under the same assumption,  $Z(i, T) \approx Z_{tr} \times (i, T)$ , the error associated with direct integration of the coagulation equation, Eq. [25], becomes

$$\epsilon_j \approx -2 \sum_{i=n_{\max}+1}^{\infty} Z(i, T)Z(j, T)K(i, j)\Delta T. \quad [32]$$

From Eq. [26], the error for all particle sizes in each time step becomes

$$E \approx -2 \sum_{j=1}^{\infty} \sum_{i=n_{\max}+1}^{\infty} Z(i, T)Z(j, T)K(i, j)\Delta T. \quad [33]$$

Then the theoretical error of the direct integration behaves like

$$E \rightarrow -2\Delta T(N^2/N_0^2). \quad [34]$$

Comparison of Eq. [31] with Eq. [34] shows clearly that the approximate equation, Eq. [24], produces less theoretical error than that expressed in Eq. [1].

## V. SUMMARY

In this work we have introduced solutions to the finite domain problem of the coagulation equation. We began by addressing the problem which arises with the difficulty to perform the integration of the coagulation equation. Since there is no analytical solution to Eq. [1] for arbitrary kernel and initial distribution, the coagulation equation, in general, has to be integrated numerically. Due to the fact that the summation of the depletion terms in Eq. [1] extends to infinity, the coagulation equation needs to be truncated at some point. However, neglecting the rest of the summation from the truncation point to infinity causes



an instability in time and an accumulation of error which cannot be ignored. Based on this dilemma, we have suggested two new approaches which take into account this finite domain problem.

The polynomial solution given in Eqs. [14] and [18] has been derived by approximating the kernel by a constant in the depletion term. This method yields an exact solution for the case of a constant kernel with any arbitrary initial distribution. As pointed out, however, the polynomial solution may not provide accurate results for variable kernels having large fluctuations from their average values. Thus, other methods must be applied.

The new numerical method to address the finite domain problem for an arbitrary kernel is to approximate the entire summation of the depletion term. In doing this, we have approximated the variable kernel by a constant only from some point  $n_{\max}$  to infinity. Therefore, in Eq. [24] we have taken into account the entire summation. This method provides desirable results by properly choosing  $n_{\max}$ . We find that relatively small values for  $n_{\max}$  yield very accurate, stable evolutions from arbitrary initial distributions. The method we have adopted is independent of which specific numerical integration method is employed in solving the "altered" coagulation equations. We find that the increase in accuracy induced by taking into effect the dominant depletion improves the accuracy considerably over the evolutions made without our method.

For any kernel, a second peak is observed when considering sufficiently narrow distributions. Indication of this phenomenon is provided with an initial gamma distribution around  $P = 5$ . The position of the second peak is almost twice that of the volume of the first peak. One expects that as the initial distribution becomes increasingly narrow, third and higher order peaks may be observed. Thus when the initial distribution gets close to a

monodisperse distribution we expect to see more peaks.

The finite domain problem is not unique to the kinetic theory of coagulation. A similar problem is shared by the kinetic theories of fragmentation, and nucleation. We expect that the infinite tail approximation discussed in this work may be profitably applied to such phenomena.

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