Sectional Representations for Simulating Aerosol Dynamics

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A general method for simulating aerosol size distribution dynamics is developed. The method, based on dividing the particle size domain into sections and dealing only with one integral quantity in each section (e.g., number, surface area, or volume), has the advantages that the integral quantity is conserved within the computational domain and coagulations between all particle sizes are properly accounted for. To demonstrate the simplicity and accuracy of the method for a practical problem, the evolution of a power plant plume aerosol undergoing coagulation is simulated.

I. INTRODUCTION

Much effort has been devoted to solving the equations that govern the particle size distribution of a coagulating aerosol (1–3). For a spatially and chemically homogeneous aerosol, the size distribution is described by the concentration of discrete particles per unit volume of fluid, n_i, $i = 1, 2, \ldots$, where i is the number of monomers in the particle and it is assumed that each particle consists of an integer multiple of monomers, e.g., molecules (3). In general, the total number of discrete particle sizes needed to simulate actual aerosols can be immense. To avoid the dimensionality problem associated with population balance equations in discrete form, the continuous version, a single integrodifferential equation, often called the coagulation equation, is used. Aside from a few special instances in which this equation may be solved analytically (4, 5), because of the complicated form of the coagulation coefficient and the complex aerosol size distributions observed in the atmosphere, it is necessary to resort to numerical solution. Virtually all general numerical solution procedures for the dynamic aerosol balance equation necessitate some form of finite sectional approximation. That is, it is necessary to approximate the virtually continuous size spectrum by a set of size classes, or sections, within which all particles are assumed to be of the same size or the functional form of the size distribution within the section is specified. By dividing the entire particle size domain into sections and dealing only with one integral quantity in each section, rather than with each n_i, the number of conservation equations required is simply equal to the number of sections.

Although so-called "size class" or "sectional" representations of aerosol balance equations have been used from time to time (6–8), no totally rigorous derivation of these representations that fully accounts for coagulations of all particle sizes is available, and a completely general framework within which such representations may be developed and assessed has not been reported. Thus, in part II we rigorously derive general sectional representations for the

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aerosol balance equations in which one may select arbitrarily the location, number, and integral quantity of interest of the aerosol for all sections. The derivation can be presented in terms of either a continuous or discrete size distribution. Although both derivations must of course lead to the same final sectional equations, we present the derivation based on the continuous distribution because of the practical aspects of determining inter- and intrasectional coagulation coefficients. For completeness, the derivation of the sectional equations from a discrete distribution is given in Appendix A.

In part III, two limiting cases of sectional equations are investigated. It is shown that the sectional equations reduce to the classical coagulation equation as the section size decreases, thereby indicating that the sectional solution should approach the exact solution as the number of sections is increased for a fixed particle size domain. The second limiting case constrains the minimum section size, which greatly simplifies the sectional equations for practical applications.

In part IV, various sectionalizations are applied to simulate the coagulation of a power plant plume aerosol. By comparing the sectional solutions to a more accurate solution, it will be shown that sectional solutions are a very practical and simple way of obtaining a fair amount of information for realistic problems if the proper sectionalization is utilized. Finally, in part V the computing requirements of sectional equations for aerosol dynamics are discussed and the advantages and disadvantages of sectional solutions are summarized.

II. GOVERNING EQUATIONS FOR A GENERAL SECTIONAL REPRESENTATION

We consider a spatially homogeneous aerosol the particles of which can be characterized by a single variable, v, which is conserved during coagulation and is usually taken to be particle volume. We assume only binary collisions occur, and the rate of coagulation of particles in the size range $[v, v + dv]$ with those in the size range $[u, u + du]$ is given by $\beta(v,u)n(v,t)n(u,t)\,dudv$, where $\beta(v,u)$ is the coagulation coefficient and $n(v,t)$ is the size distribution function, defined such that $n(v,t)dv$ is the number concentration of particles in the size range $[v, v + dv]$ at time t.

One can introduce a general property of the aerosol,

$$q(v,t) = \alpha v^{\gamma} n(v,t) \qquad [1]$$

where α and γ are constants. For example, for $\alpha = 1$ and $\gamma = 0$, $q(v,t)$ is simply equal to $n(v,t)$. If $\alpha = \pi^{1/3}6^{2/3}$ and $\gamma = 2/3$, $q(v,t)$ represents the aerosol surface area distribution, and for $\alpha = 1$ and $\gamma = 1$, $q(v,t)$ is the aerosol volume distribution.

By dividing the entire particle size domain into m arbitrary sections, one can define Q_l to be an integral quantity of aerosol in section l,

$$Q_l(t) = \int_{v_{l-1}}^{v_l} q(v,t)dv \qquad l = 1, 2, \ldots, m \qquad [2]$$

where v_{l-1} and v_l denote the volumes of the smallest and largest particles, respectively, in section l. Note that v_0 is arbitrary and the upper bound of section $l - 1$ is equal to the lower bound of section l for $l = 2, 3, \ldots, m$.

Our objective is to derive a general conservation equation for Q_l. We begin by determining the change in the property $q(v,t)$ due to each coagulation. Then by deriving expressions for the net rates by which particles are (i) added to section l, (ii) removed from section l, and (iii) remain in section l, the overall rate of change of Q_l can be determined.

Before coagulation the combined property q of two particles of volumes u and v is $\alpha(u^{\gamma} + v^{\gamma})$. After coagulation the property of the new particle formed is $\alpha(u + v)^{\gamma}$.

Thus, the change in q due to coagulation is $\alpha[(u+v)^\gamma - (u^\gamma + v^\gamma)]$. Therefore, the number of particles is reduced by one ($\alpha = 1, \gamma = 0$), and the volume of particles remains unchanged ($\alpha = 1, \gamma = 1$). Whenever a particle of volume u in section l coagulates with a particle of volume v from any lower section (one prior to l), if the new resulting particle remains in section l, Q_l is increased by $\alpha[(u+v)^\gamma - u^\gamma]$. If the new particle lies outside section l, Q_l is decreased by αu^γ.

For $l \geq 2$, the total rate of coagulation between particles in sections lower than l is given by

$$\frac{1}{2}\int_{v_0}^{v_{l-1}}\int_{v_0}^{v_{l-1}} \beta(u,v)n(u,t)n(v,t)dudv. \quad [3]$$

Only when a new particle has a volume between v_{l-1} and v_l, is it added to section l. For this reason we introduce the function

$$\theta(v_{l-1} < u + v < v_l) = \begin{cases} 1 & v_{l-1} < u + v < v_l \\ 0 & \text{otherwise.} \end{cases} \quad [4]$$

Thus, the net rate of addition of particles to section l by coagulation of particles in lower sections may be expressed as

$$\frac{1}{2}\int_{v_0}^{v_{l-1}}\int_{v_0}^{v_{l-1}} \theta(v_{l-1} < u + v < v_l) \times \beta(u,v)n(u,t)n(v,t)dudv. \quad [5]$$

The net flux of Q into section l as a result of these coagulations is therefore given by

$$\frac{1}{2}\int_{v_0}^{v_{l-1}}\int_{v_0}^{v_{l-1}} \alpha\theta(v_{l-1} < u + v < v_l)(u+v)^\gamma \times \beta(u,v)n(u,t)n(v,t)dudv. \quad [6]$$

The flux of Q into section l due to coagulation of particles from section l with those in lower sections is given by

$$\int_{v_0}^{v_{l-1}}\int_{v_0}^{v_l} \alpha\theta(u + v < v_l)[(u+v)^\gamma - u^\gamma] \times \beta(u,v)n(u,t)n(v,t)dudv \quad [7]$$

where, as above, θ(condition) is 1 if the condition is satisfied and 0 if it is not. Note that the number concentration of particles in a section cannot increase by coagulation of particles within that section with those of any other section. Thus, for $\gamma = 0$, [7] vanishes. For $\gamma = 1$, only the volume of the particle from the lower section contributes to Q_l.

The flux of Q leaving the lth section due to coagulation of particles within the lth section with those of lower sections is given by

$$\int_{v_0}^{v_{l-1}}\int_{v_{l-1}}^{v_l} \alpha\theta(u + v > v_l)u^\gamma \times \beta(u,v)n(u,t)n(v,t)dudv. \quad [8]$$

Note that only if the resulting particle size is greater than v_l is the quantity αu^γ removed from the lth section.

The flux of Q leaving the lth section due to coagulation within the lth section is given by the sum of the following two terms:

(i) For resulting particle sizes which are greater than v_l, the flux of Q leaving the section is,

$$\frac{1}{2}\int_{v_{l-1}}^{v_l}\int_{v_{l-1}}^{v_l} \alpha\theta(u + v > v_l)(u^\gamma + v^\gamma) \times \beta(u,v)n(u,t)n(v,t)dudv. \quad [9]$$

(ii) For resulting particle sizes which remain within the lth section, the loss rate of Q within the section is

$$\frac{1}{2}\int_{v_{l-1}}^{v_l}\int_{v_{l-1}}^{v_l} \alpha\theta(u + v < v_l)[u^\gamma + v^\gamma - (u+v)^\gamma]\beta(u,v)n(u,t)n(v,t)dudv. \quad [10]$$

Clearly, since v is conserved by coagulation, [10] vanishes for $\gamma = 1$, and thus no aerosol volume is lost from section l, by coagulation within the section, that does not result in a particle size greater than v_l.

Finally, for $l < m$, the flux of Q leaving section l by the coagulation of particles within section l and those of higher sections is,

$$\int_{v_l}^{v_m}\int_{v_{l-1}}^{v_l} \alpha u^\gamma \beta(u,v)n(u,t)n(v,t)dudv. \quad [11]$$

Combining the terms in [6]–[11], the sectional conservation equations for Q_l, $l = 1, 2, \ldots, m$, are

$$\frac{dQ_l}{dt} = \frac{1}{2}\int_{v_0}^{v_{l-1}}\int_{v_0}^{v_{l-1}} \alpha\theta(v_{l-1} < u + v < v_l)(u + v)^\gamma\beta(u,v)n(u,t)n(v,t)dudv$$
$$- \int_{v_0}^{v_{l-1}}\int_{v_{l-1}}^{v_l} \alpha\{\theta(u + v > v_l)u^\gamma - \theta(u + v < v_l)[(u + v)^\gamma - u^\gamma]\}\beta(u,v)n(u,t)n(v,t)dudv$$
$$- \frac{1}{2}\int_{v_{l-1}}^{v_l}\int_{v_{l-1}}^{v_l} \alpha\{\theta(u + v > v_l)(u^\gamma + v^\gamma) + \theta(u + v < v_l)[u^\gamma + v^\gamma - (u + v)^\gamma]\}$$
$$\times\ \beta(u,v)n(u,t)n(v,t)dudv - \int_{v_l}^{v_m}\int_{v_{l-1}}^{v_l} \alpha u^\gamma\beta(u,v)n(u,t)n(v,t)dudv \quad [12]$$

where the first two terms on the right hand side of Eq. [12] are evaluated only for $l > 1$, and the last term is evaluated only for $l < m$.

To obtain the contributions of the various sections to the change in Q_l, replace the integrals in Eq. [12] that range over more than one section, by a sum of integrals over each section.

$$\frac{dQ_l}{dt} = \frac{1}{2}\sum_{i=1}^{l-1}\sum_{j=1}^{l-1}\int_{v_{i-1}}^{v_i}\int_{v_{j-1}}^{v_j} \alpha\theta(v_{l-1} < u + v < v_l)(u + v)^\gamma\beta(u,v)n(u,t)n(v,t)dudv$$
$$- \sum_{i=1}^{l-1}\int_{v_{i-1}}^{v_i}\int_{v_{l-1}}^{v_l} \alpha\{\theta(u + v > v_l)u^\gamma - \theta(u + v < v_l)[(u + v)^\gamma - u^\gamma]\}$$
$$\times\ \beta(u,v)n(u,t)n(v,t)dudv$$
$$- \frac{1}{2}\int_{v_{l-1}}^{v_l}\int_{v_{l-1}}^{v_l} \alpha\{\theta(u + v > v_l)(u^\gamma + v^\gamma) + \theta(u + v < v_l)[u^\gamma + v^\gamma - (u + v)^\gamma]\}$$
$$\times\ \beta(u,v)n(u,t)n(v,t)dudv - \sum_{i=l+1}^{m}\int_{v_{l-1}}^{v_i}\int_{v_{l-1}}^{v_l} \alpha u^\gamma\beta(u,v)n(u,t)n(v,t)dudv. \quad [13]$$

The first term on the right-hand side of Eq. [13] represents all the coagulations between sections prior to section l. The second term represents all coagulations between section l and the lower sections, $l - 1, l - 2, \ldots, 1$. Coagulations within section l appear in the third term, and coagulations between section l and all the higher sections are described by the fourth term.

To express dQ_l/dt in terms of Q_i, $i = 1, 2, \ldots, m$, so as to obtain a closed set of equations for Q_l, it is necessary to introduce the fundamental approximation inherent in sectional representations. Thus, one must choose some functional form of the distribution within the sections, such that the integral quantity of interest is equal to Q_l for section l, ($l = 1, 2, \ldots, m$).

In addition to choosing a convenient functional form for the distribution, the optimal variable for characterizing particle size must be chosen. Up to this point the size variable of interest has been taken to be the particle volume v. Frequently the aerosol size distribution is desired on a size basis other than particle volume for example, particle diameter. For spherical particles all size variables of interest can be related to v, so if the size variable is denoted as x, then $x = f(v)$, where the form of f is determined by the relation of x (e.g., diameter or mass) and v.

To obtain a closed set of equations expressed in terms of x, assume that $q(v,t)$ within each section l can be given by

$$q(v,t) = \bar{q}_l(t)f'(v) \qquad [14]$$

where $f'(v) = df/dv$ and $\bar{q}_l(t)$ is a constant within each section. From Eqs. [2] and [14], [14],

$$Q_l(t) = \bar{q}_l(t)[f(v_l) - f(v_{l-1})] \qquad [15]$$

and from Eq. [1] for $v_{l-1} < v < v_l$,

$$n(v,t) = \frac{Q_l(t)f'(v)}{\alpha v^\gamma[f(v_l) - f(v_{l-1})]}. \qquad [16]$$

For $f(v) = v$, for example, Eq. [16] reduces to

$$n(v,t) = \frac{Q_l(t)}{\alpha v^\gamma(v_l - v_{l-1})}. \qquad [17]$$

Thus, the choice of both the aerosol property q, which is to be conserved, and the size variable $x = f(v)$ is available. When the choice is made, a plot of $\bar{q}_l(t)$ versus x will result in a series of step functions such that the area under each step is proportional to Q_l.

Note that one may equally as well have chosen a distribution function with $P + 1$ arbitrary constants (e.g., a Pth order polynomial), and impose a total of P continuity conditions at the ends of each section, with condition $P + 1$ obtained from Eq. [13]. Although one can continue to increase the degree of sophistication, the major objective of a sectional representation is to obtain a reasonably accurate solution, with a minimum amount of effort. Therefore, since the more accurate solution techniques do essentially use sectionalization with higher order functions (1, 2), one can thus view the sectional equations developed in this work as the lowest order solution, which requires the least amount of computation per section.[1]

Substituting Eq. [16] into Eq. [13] results in,

$$\begin{aligned}
\frac{dQ_l}{dt} &= \frac{1}{2}\sum_{i=1}^{l-1}\sum_{j=1}^{l-1} Q_iQ_j \int_{x_{i-1}}^{x_i}\int_{x_{j-1}}^{x_j} \frac{\theta(v_{l-1} < u + v < v_l)(u + v)^\gamma\beta(u,v)}{\alpha u^\gamma v^\gamma(x_i - x_{i-1})(x_j - x_{j-1})}\,dydx \\
&- \sum_{i=1}^{l-1} Q_iQ_l \int_{x_{i-1}}^{x_i}\int_{x_{l-1}}^{x_l} \frac{\{\theta(u + v > v_l)u^\gamma - \theta(u + v < v_l)[(u + v)^\gamma - u^\gamma]\}\beta(u,v)}{\alpha u^\gamma v^\gamma(x_i - x_{i-1})(x_l - x_{l-1})}\,dydx \\
&- \frac{1}{2}Q_l^2 \int_{x_{l-1}}^{x_l}\int_{x_{l-1}}^{x_l} \frac{\{\theta(u + v > v_l)(u^\gamma + v^\gamma) + \theta(u + v < v_l)[u^\gamma + v^\gamma - (u + v)^\gamma]\}\beta(u,v)}{\alpha u^\gamma v^\gamma(x_l - x_{l-1})^2}\,dydx \\
&- Q_l \sum_{i=l+1}^{m} Q_i \int_{x_{i-1}}^{x_i}\int_{x_{l-1}}^{x_l} \frac{u^\gamma\beta(u,v)}{\alpha u^\gamma v^\gamma(x_i - x_{i-1})(x_l - x_{l-1})}\,dydx \qquad [18]
\end{aligned}$$

where $x_i = f(v_i)$, $v = f^{-1}(x)$, and $u = f^{-1}(y)$. Using the definitions of the sectional coagulation coefficients as given in Table I, Eq. [18] can be reduced to the final general sectional equations,

$$\frac{dQ_l}{dt} = \frac{1}{2}\sum_{i=1}^{l-1}\sum_{j=1}^{l-1} {}^1\bar{\beta}_{i,j,l}Q_iQ_j - Q_l\sum_{i=1}^{l-1} {}^2\bar{\beta}_{i,l}Q_i - \frac{1}{2}{}^3\bar{\beta}_{l,l}Q_l^2 - Q_l\sum_{i=l+1}^{m} {}^4\bar{\beta}_{i,l}Q_i \qquad [19]$$

where the first two terms on the right-hand side of Eq. [19] are evaluated only for $l \geq 2$ and the last term is evaluated only for $l < m$.

Having developed the general sectional equations, a few words are in order before we proceed to discuss limiting cases and

[1] The addition of continuity constraints usually requires the solution of a set of algebraic equations in addition to the differential equations as given in Eq. [13].

TABLE I

Inter- and Intrasectional Coagulation Coefficients

Symbol	Remarks	Coefficient[a]
${}^1\bar{\beta}_{i,j,l}$	$2 \le l \le m$; $1 \le i < l$; $1 \le j < l$; ${}^1\bar{\beta}_{i,j,l} = {}^1\bar{\beta}_{j,i,l}$	$\int_{x_{i-1}}^{x_i}\int_{x_{j-1}}^{x_j} \frac{\theta(v_{l-1} < u + v < v_l)(u+v)^\gamma \beta(u,v)}{\alpha u^\gamma v^\gamma (x_i - x_{i-1})(x_j - x_{j-1})} dydx$
${}^2\bar{\beta}_{i,l}$	$2 \le l \le m$; $i < l$; ${}^2\bar{\beta}_{i,l} \ne {}^2\bar{\beta}_{l,i}$	$\int_{x_{i-1}}^{x_i}\int_{x_{l-1}}^{x_l} \frac{[\theta(u + v > v_l)u^\gamma - \theta(u + v < v_l)((u+v)^\gamma - u^\gamma)]\beta(u,v)}{\alpha u^\gamma v^\gamma (x_i - x_{i-1})(x_l - x_{l-1})} dydx$
${}^3\bar{\beta}_{l,l}$	$1 \le l \le m$	$\int_{x_{l-1}}^{x_l}\int_{x_{l-1}}^{x_l} \frac{[\theta(u + v > v_l)(u^\gamma + v^\gamma) + \theta(u + v < v_l)[(u^\gamma + v^\gamma) - (u+v)^\gamma]]\beta(u,v)}{\alpha u^\gamma v^\gamma (x_l - x_{l-1})^2} dydx$
${}^4\bar{\beta}_{i,l}$	$1 \le l < m$; $i > l$; ${}^4\bar{\beta}_{i,l} \ne {}^4\bar{\beta}_{l,i};\ \gamma > 0$; ${}^4\bar{\beta}_{i,l} = {}^4\bar{\beta}_{l,i};\ \gamma = 0$	$\int_{x_{i-1}}^{x_i}\int_{x_{l-1}}^{x_l} \frac{u^\gamma \beta(u,v)}{\alpha u^\gamma v^\gamma (x_i - x_{i-1})(x_l - x_{l-1})} dydx$

[a] $x_i = f(v_i)$, $u = f^{-1}(y)$, $v = f^{-1}(x)$.

applications of Eq. [19]. First, note that Eq. [19] is of a form such that any quantity that is a moment of the distribution can be conserved. However, for most applications one is primarily concerned with the behavior of the zeroth and first moments, i.e., the total number and volume of aerosol per unit volume of fluid, respectively. Thus, α will usually be 1 and γ either 0 or 1. Similarly, one is usually interested in the shape of the number and volume distributions as plotted versus $\log_{10}(D/1\ \mu\text{m})$, where D is the particle diameter in microns. Thus, $f(v)$, for spherical particles will often be given as,

$$f(v) = x = \log_{10}\,[(6v/\pi)^{1/3}/1\ \mu\text{m}]. \quad [20]$$

Second, note that although the derivation of the general sectional equations was facilitated by the use of a discontinuous θ function, for most applications of practical interest it will be shown that the inter- and intrasectional coagulation coefficients given in Table I can be simply expressed without a θ function. Furthermore, in Appendix B, exact, analytical expressions for some of the inter- and intrasectional coagulation coefficients for Brownian coagulation are developed for those cases in which the θ function is not used.

Finally, we note that the coefficients in Table I are exactly defined mathemathical quantities, determined by the choice of sectionalization, and no corrections are required to determine the number of particles crossing section boundaries by coagulation.

III. LIMITING CASES OF SECTIONAL EQUATIONS

A. Reduction to the Classical Coagulation Equation

The sectional equations derived in part II are not models, but an approximate form of the coagulation equation. However, before any approximate equations can be applied, one must demonstrate that the solution to the approximate equations approaches the exact solution as one increases the degree of approximation. Clearly, the limiting case of sectionalization would be a single particle size in each section. For that case it has been shown that the distribution function can be represented by a constant within each section (3). To show that Eq. [19] reduces to the coagulation equation let $f(v) = v$, $\alpha = 1$, $\gamma = 0, dv = v_i - v_{i-1} = v_0$ for $i = 1, 2, \ldots, m$ and substitute Eq. [17] into Eq. [18]. Then by changing the order of integration for the second and fourth terms on the right-hand side of Eq. [18] we have,

$$\begin{aligned}\frac{d[n(v_l,t)dv]}{dt} &= \frac{1}{2}\sum_{i=1}^{l-1}\int_{v_{i-1}}^{v_i}\sum_{j=1}^{l-1}\int_{v_{j-1}}^{v_j}\theta(v_{l-1} < u + v < v_l)\beta(u,v)n(v_i,t)n(v_j,t)dudv \\ &\quad - n(v_l,t)\int_{v_{l-1}}^{v_l}\sum_{i=1}^{l-1}\int_{v_{i-1}}^{v_i}\theta(u + v > v_l)\beta(u,v)n(v_i,t)dudv \\ &\quad - \frac{n(v_l,t)}{2}\int_{v_{l-1}}^{v_l}\int_{v_{l-1}}^{v_l}[2\theta(u + v > v_l) + \theta(u + v < v_l)]\beta(u,v)n(v_l,t)dudv \\ &\quad - n(v_l,t)\int_{v_{l-1}}^{v_l}\sum_{i=l+1}^{m}\int_{v_{i-1}}^{v_i}\beta(u,v)n(v_i,t)dudv \qquad [21]\end{aligned}$$

where $n(v_i,t)$ is constant in the regions $[v_{i-1}, v_i]$ for $i = 1, 2, \ldots, m$. To sum the integrals note that

$$\sum_{i=1}^{l-1}\int_{v_{i-1}}^{v_i} n(v_i,t)du = \int_{v_0}^{v_{l-1}} n(u,t)du. \qquad [22]$$

Also note that in the second term on the right-hand side of Eq. [21] the minimum value of v over the outer integration is $v_{l-1} = v_l - v_0$, and the minimum value of u over the inner integration is v_0. Therefore, $\theta(u + v > v_l) = 1$ except at $u = v_0$ and $v = v_{l-1}$. However, for the purposes of integration this point can be neglected. For the third term on the right-hand side of Eq. [21], the integration is over one particle size, thus $u + v \geq v_l$, $\theta(u + v < v_l) = 0$, and $\theta(u + v > v_l) = 1$ (except for the point $u = v = v_0$, which can be neglected). Therefore Eq. [21] reduces to,

$$\begin{aligned}\frac{d[n(v_l,t)dv]}{dt} &= \frac{1}{2}\int_{v_0}^{v_{l-1}}\int_{v_0}^{v_{l-1}}\theta(v_{l-1} < u + v < v_l)\beta(u,v)n(u,t)n(v,t)dudv \\ &\quad - n(v_l,t)\int_{v_{l-1}}^{v_l}\int_{v_0}^{v_{l-1}}\beta(u,v)n(u,t)dudv - n(v_l,t)\int_{v_{l-1}}^{v_l}\int_{v_{l-1}}^{v_l}\beta(u,v)n(u,t)dudv \\ &\quad - n(v_l,t)\int_{v_{l-1}}^{v_l}\int_{v_l}^{v_m}\beta(u,v)n(u,t)dudv. \qquad [23]\end{aligned}$$

The first term on the right-hand side of Eq. [23] vanishes unless a particle in the size range of v_l is formed. Therefore, v is given by $v_l - u$ as u varies from v_0 to $v_{l-1} = v_l - v_0$. Combining the last three terms in Eq. [23] results in

$$\begin{aligned}\frac{d[n(v_l,t)dv]}{dt} &= \frac{dv}{2}\int_{v_0}^{v_l - v_0}\beta(u, v_l - u) \\ &\quad \times n(u,t)n(v_l - u, t)du \\ &\quad - n(v_l,t)dv\int_{v_0}^{v_m}\beta(u,v)n(u,t)du. \qquad [24]\end{aligned}$$

TABLE II

Inter- and Intrasectional Coagulation Coefficients with Geometric Constraint ($v_{i+1} \geq 2v_i$, $i = 0, 1, 2, \ldots, m - 1$)

Symbol	Remarks	Coefficient[a]
${}^1\bar{\beta}_{i,j,l}$	$i < l - 1$ $j < l - 1$	0
${}^1\bar{\beta}_{i,l-1,l}$	$2 \leq l \leq m$ $i < l - 1$	$\int_{x_{i-1}}^{x_i} \int_{f(v_{l-1}-v)}^{x_{l-1}} \frac{(u+v)^\gamma \beta(u,v)}{\alpha u^\gamma v^\gamma (x_i - x_{i-1})(x_{l-1} - x_{l-2})} dydx$
	$2 \leq l \leq m$ $i = l - 1$	$\int_{x_{i-1}}^{f(v_i - v_{i-1})} \int_{f(v_{l-1}-v)}^{x_{l-1}} \frac{(u+v)^\gamma \beta(u,v)}{\alpha u^\gamma v^\gamma (x_i - x_{i-1})(x_{l-1} - x_{l-2})} dydx + \int_{f(v_i - v_{l-1})}^{x_i} \int_{x_{l-2}}^{x_{l-1}} \frac{(u+v)^\gamma \beta(u,v)}{\alpha u^\gamma v^\gamma (x_i - x_{i-1})(x_{l-1} - x_{l-2})} dydx$
${}^2\bar{\beta}_{i,l}$	$2 \leq l \leq m$ $i < l$	$\int_{x_{i-1}}^{x_i} \int_{f(v_l-v)}^{x_l} \frac{u^\gamma \beta(u,v)}{\alpha u^\gamma v^\gamma (x_i - x_{i-1})(x_l - x_{l-1})} dydx - \int_{x_{i-1}}^{x_i} \int_{x_{l-1}}^{f(v_l-v)} \frac{[(u+v)^\gamma - u^\gamma] \beta(u,v)}{\alpha u^\gamma v^\gamma (x_i - x_{i-1})(x_l - x_{l-1})} dydx$
${}^3\bar{\beta}_{l,l}$	$1 \leq l \leq m$	$\int_{x_{l-1}}^{f(v_l - v_{l-1})} \int_{f(v_l-v)}^{x_l} \frac{(u^\gamma + v^\gamma) \beta(u,v)}{\alpha u^\gamma v^\gamma (x_l - x_{l-1})^2} dydx + \int_{f(v_l - v_{l-1})}^{x_l} \int_{x_{l-1}}^{x_l} \frac{(u^\gamma + v^\gamma) \beta(u,v)}{\alpha u^\gamma v^\gamma (x_l - x_{l-1})^2} dydx + \int_{x_{l-1}}^{f(v_l - v_{l-1})} \int_{x_{l-1}}^{f(v_l-v)} \frac{[u^\gamma + v^\gamma - (u+v)^\gamma] \beta(u,v)}{\alpha u^\gamma v^\gamma (x_l - x_{l-1})^2} dydx$
${}^4\bar{\beta}_{i,l}$	$1 \leq l < m$ $l < i$	$\int_{x_{i-1}}^{x_i} \int_{x_{l-1}}^{x_l} \frac{u^\gamma \beta(u,v)}{\alpha u^\gamma v^\gamma (x_i - x_{i-1})(x_l - x_{l-1})} dydx$

[a] $x_i = f(v_i)$, $u = f^{-1}(y)$, $v = f^{-1}(x)$. Note that the first two terms of ${}^3\bar{\beta}_{l-1,l-1}$ are equal to ${}^1\bar{\beta}_{l-1,l-1,l}$.

Dropping the subscript l and dividing by dv results in the continuous form of the classical coagulation equation as $v_0 \to 0$. Thus, as the sectional equations approach the coagulation equation, the solution to the sectional equations should approach the solution to the coagulation equation.

B. Geometric Sectionalization

Although the derivation of the general sectional equations was facilitated by the use of a discontinuous θ function, the particle size range of interest is usually so large that one can impose a geometric constraint on the section boundaries (i.e., $v_i \geq 2v_{i-1}$, $i = 1, 2, \ldots, m$), without greatly limiting most applications of the equations. This condition specifies that at least one of the coagulating particles from sections prior to section l must be in section $l - 1$ to form a particle in section l. Therefore, ${}^1\bar{\beta}_{i,j,l} = 0$ for $i < l - 1$ and $j < l - 1$ as given in Table II. For $j = l - 1$ and $i < l - 1$, to form a particle in section l, a particle of size v in section i must coagulate with a particle in section $l - 1$ of size $v_{l-1} - v$ or greater. Thus, the lower limit of the inner integration given to Table II for ${}^1\bar{\beta}_{i,l-1,l}$ is $f(v_{l-1} - v)$. Since the geometric constraint imposes that for $2v_{l-1} \leq v_l$, thus $v_i + v_{l-1} < v_l$ for $i < l - 1$ and all resulting particles larger than v_{l-1} will be in section l and in no higher sections. For ${}^1\bar{\beta}_{l-1,l-1,l}$ the upper limit of the outer integration of the first term is $f(v_{l-1} - v_{l-2})$, since particles larger than $v_{l-1} - v_{l-2}$ would force the lower limit of the inner integration below x_{l-2}. The remaining outer integration is given by the second term for ${}^1\bar{\beta}_{l-1,l-1,l}$.

For ${}^2\bar{\beta}_{i,l}$, a particle of size v in section i will remove all particles larger than $v_l - v$ from section l. Therefore, the lower limit of the inner integration for the first term is $f(v_l - v)$. Particles smaller than $v_l - v$ will remain in section l and thus $f(v_l - v)$ is the upper limit of the inner integration of the second term. Because of the geometric constraint $v_l - v_{l-1} \geq v_{l-1}$, and thus $f(v_l - v) \geq x_{l-1}$, which indicates that the inner integration of the first term must be within the lth section.

For ${}^3\bar{\beta}_{l,l}$ the integration limits of the first two terms given in Table II are derived by the same reasoning used in obtaining ${}^1\bar{\beta}_{l-1,l-1,l}$. The reasoning for the upper limit of the inner integration of the third term is the same as that used for the second term for ${}^2\bar{\beta}_{i,l}$. The upper limit of the outer integration of the third term for ${}^3\bar{\beta}_{l,l}$ ensures that the upper limit of the inner integration will not extend below x_{l-1}. Finally we note that ${}^4\bar{\beta}_{i,l}$ is not affected by the geometric constraint.

Because of the geometric constraint, $v_m \geq 2^m v_0$, thus given the computational domain $[v_0, v_m]$, the maximum number of sections is given by

$$m = \frac{\log\left(\dfrac{v_m}{v_0}\right)}{\log(2)}. \quad [25]$$

One can of course use fewer sections and still use Table II to calculate the inter- and intrasectional coefficients, as long as the geometric constraint is satisfied.

IV. APPLICATIONS

To demonstrate the convergence and simplicity of sectional equations for practical problems, the evolution of the size distribution of a power plant plume aerosol undergoing coagulation was computed using a spline technique (2) and the sectional equations. For a representative initial distribution, a trimodal distribution as given by Whitby (9) for the Labadie power plant plume was used. Since the distributions are usually expressed in terms of particle diameter on a logarithmic scale, $f(v)$ was determined from Eq. [20]. The Fuchs–Phillips coagulation coefficient (10) for spherical particles with a density of 1.0 g/cm^3 in air at 298°K was used in all the calculations. Although other phenomena, such as particle growth, production, and removal mechanisms can also be incorporated into the sectional equations, for simplicity, only coagulation was considered since it introduces the greatest numerical difficulties and the evolution of the distribution in the absence of coagulation can be solved by other methods (11). Since no exact solution of the coagulation equation for the initial distribution and coagulation coefficient used in the calculations has been reported, the spline solution will be taken as being correct for the purposes of comparison, since the technique has been shown to be accurate (2).[2]

Figure 1 shows the evolution of the number distribution for a 4 hr simulation. As expected, the smaller particles are scavenged by the larger particles, therefore we note the decrease in the spline solution for small particles. Using $\alpha = 1$, $\gamma = 0$, and only three sections, the sectional solution provides an unacceptable gross description of the aerosol as shown in Fig. 1. The distribution as determined by the sectional solution increases significantly for particles larger than 0.794 μm in diameter which is in qualitative disagreement with the spline solution. Clearly, more sections are

[2] It is important to monitor the so-called "finite domain errors," by checking that $\int_{v_0}^{v_m} vn(v,t)dv$ is conserved during the computations (2). For this problem the spline solution finite domain error was less than 0.004%.

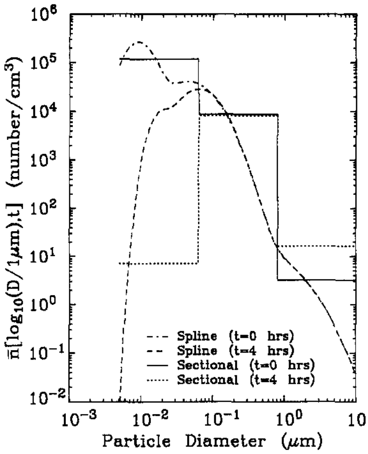

FIG. 1. Comparison of the spline and sectional solution (using three logarithmically spaced sections), for the evolution of the number distribution $\bar{n} = n(v,t)dv/d[\log_{10}(D/1\ \mu m)]$, of an aerosol undergoing Brownian coagulation. $\alpha = 1$, $\gamma = 0$, and $f(v) = \log_{10}[(6v/\pi)^{1/3}/1\ \mu m]$.

required to obtain a meaningful solution. Similarly, the volume distribution shown in Fig. 2 using only three sections and $\alpha = \gamma = 1$ does not provide an acceptable description of the aerosol.

Since the sectional solution should approach the exact solution as the number of sections is increased, the evolution of the same initial distribution as shown in Fig. 1 and was simulated using 10 sections. As shown in Fig. 3, the sectional solution for the number distribution is clearly more accurate than that shown in Fig. 1. We note that the sectional solution in Fig. 3 is in excellent agreement with the more detailed and accurate spline solution. Similarly, the volume distributions shown in Fig. 4 for 10 sections is in excellent agreement with the spline solution and is clearly more accurate than the sectional solution shown in Fig. 2.

V. CONCLUSIONS

A. Computing Requirements of Sectional Equations

After selecting the location, number, and integral quantity of interest for the sections, essentially two major computational steps are required to obtain the evolution of the size distribution. First, the sectional coagulation coefficients as given in Table I or Table II must be evaluated. Second, the system of first-order ordinary differential equations as given in Eq. [19] must be integrated. For evaluating the sectional coagulation coefficients, it is noted in Appendix B that for Brownian coagulation some of the integrals can be evaluated analytically. Even in cases for which analytical expressions cannot be obtained, standard techniques are available for numerical integration.[3]

The total number of sectional coefficients can be obtained as follows. For section l (where $l > 1$), there are $l(l-1)/2$ coefficients for ${}^1\bar{\beta}_{i,j,l}$ (since ${}^1\bar{\beta}_{i,j,l} = {}^1\bar{\beta}_{j,i,l}$). Therefore for m sections a total of

$$\sum_{l=2}^{m} \frac{l(l-1)}{2} = \frac{(m+1)(m-1)m}{6} \qquad [26]$$

coefficients for ${}^1\bar{\beta}$ must be computed. Only

[3] In cases for which numerical integration is required there is little advantage in imposing the geometric constraint to simplify the integration.

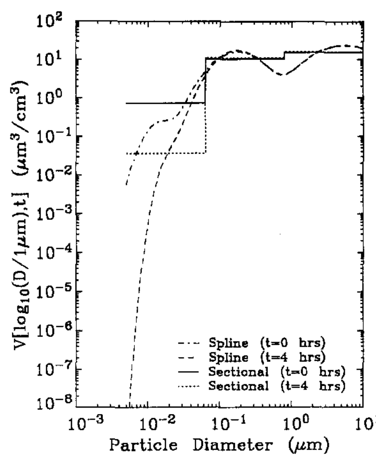

FIG. 2. Comparison of the spline and sectional solution (using three logarithmically spaced sections), for the evolution of the volume distribution $V = (\pi D^3/6)n(v,t)dv/d[\log_{10}(D/1\ \mu m)]$ of an aerosol undergoing Brownian coagulation. $\alpha = \gamma = 1$ and $f(v) = \log_{10}[(6v/\pi)^{1/3}/1\ \mu m]$.

$m(m-1)/2$ coefficients must be computed for both ${}^2\bar{\beta}$ and ${}^4\bar{\beta}$, and m coefficients are required for ${}^3\bar{\beta}$. Thus, the total number of sectional coefficients is,

$$\frac{m^3 + 6m^2 - m}{6}. \qquad [27]$$

However, if one imposes the geometrical constraint there are only $m(m-1)/2$ nonzero coefficients for ${}^1\bar{\beta}$ and thus the total number of coefficients reduces to,

$$\frac{3m^2 - m}{2}. \qquad [28]$$

Although [27] is the total number of sectional coefficients, even if the geometric constraint is not imposed some coefficients for ${}^1\bar{\beta}$ may be zero and thus [27] is the maximum number of nonzero coefficients. Therefore, [27] and [28] are the upper and lower bounds, respectively, on the number of nonzero sectional coefficients.

B. Advantages and Disadvantages of Sectional Equations

Although sectional solutions are relatively straightforward, the advantages and disadvantages should be considered before choosing it over other techniques. As shown in Table III, the major preliminary calculation of sectional solutions involves the computation of sectional coefficients. For comparison, a spline solution merely requires fitting the initial distribution and evaluating β at the quadrature points. To assess the relative computational effort of the two techniques for the same number of differential equations, we note that in part IV of this work 46 differential equations were used for the spline solution. Since the computational domain was [0.005–10.0 μm] in particle diameter, the maximum number of sections that can be used for a geometric sectionalization as determined by Eq. [25] is 32. However, since 46 differential equations would exceed this maximum, the maximum number of nonzero sectional coefficients required is determined from [27] and is equal to 18,331. Therefore, for the same number of differential equations it is generally easier to initiate a spline solution.[4] However, since

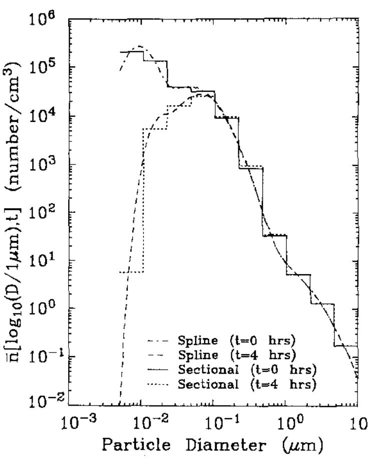

FIG. 3. Comparison of the spline and sectional solution (using 10 logarithmically spaced sections), for the evolution of the number distribution $\bar{n} = n(v,t)dv/d[\log_{10}(D/1\ \mu\text{m})]$, of an aerosol undergoing Brownian coagulation. $\alpha = 1$, $\gamma = 0$, and $f(v) = \log_{10}[(6v/\pi)^{1/3}/1\ \mu\text{m}]$.

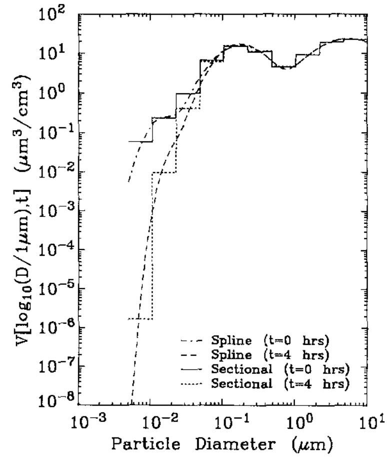

FIG. 4. Comparison of the spline and sectional solution (using 10 logarithmically spaced sections) for the evolution of the volume distribution $V = (\pi D^3/6)nc(v,t)dv/d[\log_{10}(D/1\ \mu\text{m})]$ of an aerosol undergoing Brownian coagulation. $\alpha = \gamma = 1$ and $f(v) = \log_{10}[(6v/\pi)^{1/3}/1\ \mu\text{m}]$.

[4] Although the number of sectional coefficients increases rapidly with the number of sections, the section size decreases and the variation of $\beta(u,v)$ between particles of two sections may be small

TABLE III

Comparison of Sectional and Spline Solutions

Category	Sectional	Spline (2)
1. Preliminary calculations	Determine initial concentration in each section. Evaluation of sectional coefficients. (Rapid increase of computational effort with increasing number of differential equations)	Initial curve fit. Evaluate $\beta(u,v)$ at quadrature points. (Relatively moderate increase of computational effort with increasing number of differential equations)
2. Time integration requirements	Relatively small for a reasonable number of sections	Curve fitting and 2 one-dimensional quadratures required each time step
3. Solution characteristics	Discontinuous	Continuous function and continuous up to and including the pth derivative for a spline of order $p + 1$
4. Programming requirements	Two-dimensional quadrature and differential equation routines	Curve fitting, one-dimensional quadrature and differential equation routines
5. Areas of difficulty	None encountered to date	Except for always positive spline functions, curve fitting inaccuracies may result in a negative distribution between grid points for distributions that are sensitive to small variations in particle size

the sectional coefficients are independent of time and the distribution, once computed they can be used for other problems which have the same α, γ, $f(v)$, $\beta(u,v)$, and location and number of sections.

Once the sectional coefficients have been determined, it is relatively simple to substitute into Eq. [19] to solve for Q_l. In contrast, a spline solution requires repeated quadratures and curve fitting. For example, using m differential equations, a cubic spline such as used in part IV, requires repeated solution of a $(m - 2)$-dimensional tridiagonal linear system of algebraic equations. However, as shown in the third category of Table III, the resulting cubic spline solution is continuous and twice continuously differentiable, whereas the sectional solution is discontinuous. A linear spline, however, is only continuous, but would not require the solution to a set of algebraic equations. Both sectional and spline techniques use standard algorithms, but programming a sectional solution is simpler because no interpolations or quadratures are required for each time step. Finally, we note from Table III that a sectional solution avoids the possibility of difficulties in fitting a rapidly varying function.

enough such that $\beta(u,v)$ is practically constant. One can then remove $\beta(u,v)$ from the integrand in Tables I and II and simplify the calculation. However, one still has to contend with the large array of sectional coefficients. In comparison, the computer time and storage requirements for evaluating β at the quadrature points is usually less than that for determining sectional coefficients.

APPENDIX A. DERIVATION OF THE SECTIONAL EQUATIONS FROM THE DISCRETE DISTRIBUTION

In this Appendix the derivation of the sectional equations from a discrete distribution $n_i(t)$, where i is an integer number of monomer units in each aerosol particle, and n_i is the concentration of $i$mers per unit volume of the fluid is presented.

As in the continuous approach, let

$$q_i(t) = \alpha i^{\gamma} n_i(t) \qquad \text{[A-1]}$$

and divide the entire size domain into m arbitrary sections. The number of monomers in the smallest and largest particles in the lth section is denoted by $k_{l-1} + 1$ and k_l respectively, where $k_0 = 0$. In a discrete representation, Q_l, the integral quantity of the aerosol in section l, is given by

$$Q_l(t) = \sum_{i=k_{l-1}+1}^{k_l} \alpha i^\gamma n_i(t) \qquad l = 1, 2, \ldots, m. \qquad \text{[A-2]}$$

Using the above definitions, the general conservation equation for $Q_l(t)$ will be expressed in discrete form.

Before coagulation of an $i$mer with a $j$mer the combined property $q_i + q_j$ of the two particles is $\alpha(i^\gamma + j^\gamma)$. After coagulation the property q_{i+j} of the new formed particle is $\alpha(i + j)^\gamma$. Thus, the change in q due to coagulation is $\alpha[(i + j)^\gamma - (i^\gamma + j^\gamma)]$. Whenever an $i$mer in section l coagulates with a $j$mer from any lower section prior to l, if the new resulting particle remains in section l, Q_l is increased by $\alpha[(i + j)^\gamma - i^\gamma]$. If the new particle lies outside of section l, Q_l is decreased by αi^γ. If an $i$mer and a $j$mer both from sections prior to section l, form a new particle which is added to section l, Q_l is increased by $\alpha(i + j)^\gamma$.

The net rate of addition of particles to section l by coagulation of particles in lower sections may be expressed as

$$\frac{1}{2}\sum_{i=1}^{k_{l-1}}\sum_{j=1}^{k_{l-1}} \theta(k_{l-1} < i + j \le k_l) \times \beta_{i,j}n_i(t)n_j(t) \qquad \text{[A-3]}$$

where $\beta_{i,j}$ is the kinetic coefficient of coagulation of two particles containing i and j monomers, respectively, and as in the continuous approach the function θ(condition), is equal to 1 if the condition is satisfied and 0 if it is not. Thus, the net flux of Q into section l as a result of these coagulations is given by

$$\frac{1}{2}\sum_{i=1}^{k_{l-1}}\sum_{j=1}^{k_{l-1}} \alpha\theta(k_{l-1} < i + j \le k_l)(i + j)^\gamma \times \beta_{i,j}n_i(t)n_j(t). \qquad \text{[A-4]}$$

The flux of Q leaving section l due to coagulation of particles from section l with those in lower sections is given by

$$\sum_{i=1}^{k_{l-1}}\sum_{j=k_{l-1}+1}^{k_l} \alpha\theta(i + j > k_l)j^\gamma \times \beta_{i,j}n_i(t)n_j(t). \qquad \text{[A-5]}$$

The increase in Q_l due to coagulation of particles from section l with those in lower sections is

$$\sum_{i=1}^{k_{l-1}}\sum_{j=k_{l-1}+1}^{k_l} \alpha\theta(i + j \le k_l)[(i + j)^\gamma - j^\gamma] \times \beta_{i,j}n_i(t)n_j(t). \qquad \text{[A-6]}$$

The flux of Q leaving the lth section due to coagulation of particles within the lth section is given by the sum of the following two terms,

$$\frac{1}{2}\sum_{i=k_{l-1}+1}^{k_l}\sum_{j=k_{l-1}+1}^{k_l} \alpha\theta(i + j > k_l)(i^\gamma + j^\gamma) \times \beta_{i,j}n_i(t)n_j(t) + \frac{1}{2}\sum_{i=k_{l-1}+1}^{k_l}\sum_{j=k_{l-1}+1}^{k_l} \alpha\theta(i + j \le k_l) \times [i^\gamma + j^\gamma - (i + j)^\gamma]\beta_{i,j}n_i(t)n_j(t) \qquad \text{[A-7]}$$

where the first term is the flux of Q leaving the lth section for the new particles which are outside of section l, and the second term is for new particles that remain within section l.

Particles are also removed from section l by all coagulations with particles of the higher sections (i.e., sections $l + 1$, $l + 2$, . . . , m). Hence, the rate of removal of Q from the lth section by scavenging of particles in higher sections is given by

$$\sum_{i=k_l+1}^{k_m}\sum_{j=k_{l-1}+1}^{k_l} \alpha j^\gamma\beta_{i,j}n_i(t)n_j(t). \qquad \text{[A-8]}$$

Finally, by combining the terms [A-4] to [A-8], the sectional conservation equations for Q_l, $l = 1, 2, 3, \ldots, m$ are,

$$\frac{dQ_l}{dt} = \frac{1}{2}\sum_{i=1}^{k_{l-1}}\sum_{j=1}^{k_{l-1}} \alpha\theta(k_{l-1} < i + j \le k_l)(i+j)^\gamma \beta_{i,j} n_i(t) n_j(t) - \sum_{i=1}^{k_{l-1}}\sum_{j=k_{l-1}+1}^{k_l} \alpha\{\theta(i+j > k_l)j^\gamma$$
$$- \theta(i+j \le k_l)[(i+j)^\gamma - j^\gamma]\}\beta_{i,j} n_i(t) n_j(t) - \frac{1}{2}\sum_{i=k_{l-1}+1}^{k_l}\sum_{j=k_{l-1}+1}^{k_l} \alpha\{\theta(i+j > k_l)(i^\gamma + j^\gamma)$$
$$+ \theta(i+j \le k_l)[i^\gamma + j^\gamma - (i+j)^\gamma]\}\beta_{i,j} n_i(t) n_j(t) - \sum_{i=k_l+1}^{k_m}\sum_{j=k_{l-1}+1}^{k_l} \alpha j^\gamma \beta_{i,j} n_i(t) n_j(t) \quad \text{[A-9]}$$

where the first two terms on the right-hand side of Eq. [A-9] are evaluated only for $l \ge 2$, and the last term is evaluated only for $l < m$.

To express dQ_l/dt in terms of Q_i, $i = 1, 2, \ldots, m$, the summations in Eq. [A-9] are expanded and the terms are resummed using the bounds of each section as the limits of the summations. Then, it is necessary to introduce the fundamental approximation inherent in sectional representations; i.e., one must choose some functional form of the distribution within the sections, such that the integral quantity of interest is equal to Q_l for section l, $l = 1, 2, \ldots, m$, e.g.,

$$n_i(t) = \frac{Q_l(t)}{\alpha i^\gamma (k_l - k_{l-1})}. \quad \text{[A-10]}$$

Substituting Eq. [A-10] into Eq. [A-9] results in the discrete sectional equations,

$$\frac{dQ_l}{dt} = \frac{1}{2}\sum_{r=1}^{l-1}\sum_{p=1}^{l-1} {}^1\bar{\beta}_{r,p,l} Q_r Q_p - Q_l \sum_{r=1}^{l-1} {}^2\bar{\beta}_{r,l} Q_r - \frac{{}^3\bar{\beta}_{l,l} Q_l^2}{2} - Q_l \sum_{r=l+1}^{m} {}^4\bar{\beta}_{r,l} Q_r \quad \text{[A-11]}$$

where the inter- and intrasectional coagulation coefficients are defined in Table A-I. Notice that Eq. [A-11] is essentially identical to Eq. [19], except that for the discrete representation the integrals are replaced by

TABLE A-I

Inter- and Intrasectional Coagulation Coefficients for the Discrete Representation

Symbol	Remarks	Coefficient
${}^1\bar{\beta}_{r,p,l}$	$2 \le l \le m$ $r < l$ $p < l$	$\sum_{i=k_{r-1}+1}^{k_r}\sum_{j=k_{p-1}+1}^{k_p} \frac{\theta(k_{l-1} < i + j \le k_l)(i+j)^\gamma \beta_{i,j}}{\alpha i^\gamma j^\gamma (k_r - k_{r-1})(k_p - k_{p-1})}$
${}^2\bar{\beta}_{r,l}$	$2 \le l \le m$ $r < l$	$\sum_{i=k_{r-1}+1}^{k_r}\sum_{j=k_{l-1}+1}^{k_l} \frac{[\theta(i+j > k_l)j^\gamma - \theta(i+j \le k_l)[(i+j)^\gamma - j^\gamma]]\beta_{i,j}}{\alpha i^\gamma j^\gamma (k_r - k_{r-1})(k_l - k_{l-1})}$
${}^3\bar{\beta}_{l,l}$	$1 \le l \le m$	$\sum_{i=k_{l-1}+1}^{k_l}\sum_{j=k_{l-1}+1}^{k_l} \frac{[\theta(i+j > k_l)(i^\gamma + j^\gamma) + \theta(i+j \le k_l)[i^\gamma + j^\gamma - (i+j)^\gamma]]\beta_{i,j}}{\alpha i^\gamma j^\gamma (k_l - k_{l-1})^2}$
${}^4\bar{\beta}_{r,l}$	$1 \le l < m$ $l < r$	$\sum_{i=k_{r-1}+1}^{k_r}\sum_{j=k_{l-1}+1}^{k_l} \frac{j^\gamma \beta_{i,j}}{\alpha i^\gamma j^\gamma (k_l - k_{l-1})(k_r - k_{r-1})}$

summations. Also note that the first two terms on the right-hand side of Eq. [A-11] are evaluated only for $l > 1$ and the last term is evaluated only for $l < m$.

To show that Eq. [A-11] reduces to the discrete form of the classical coagulation equation as the number of particle sizes in each section reduces to one, let $\alpha = 1$, $\gamma = 0$, and $k_l - k_{l-1} = 1$ for $l = 1, 2, \ldots, m$ (which implies that $k_l = l$ since $k_0 = 0$). Then the first term on the right-hand side of Eq. [A-11] vanishes except for $i + j = l$. Thus, only the summation from $i = 1$ to $l - 1$ is required since $j = l - i$. For the second term on the right-hand side of Eq. [A-11], $(i + j)^\gamma - j^\gamma = 0$ and since the summation on j is only for $j = l$, $\theta(i + j > k_l) = 1$. In the third term both summations are only over the particle size l. Therefore, $\theta(i + j > k_l) = 1$ and $\theta(i + j \leq k_l) = 0$. Finally, for the last term the summation over j is only for $j = l$. Thus we have

$$\frac{dn_l(t)}{dt} = \frac{1}{2}\sum_{i=1}^{l-1} \beta_{i,l-i} n_i(t) n_{l-i}(t) - \sum_{i=1}^{l-1} \beta_{i,l} n_i(t) n_l(t) - \frac{1}{2}[2\beta_{l,l} n_l(t) n_l(t)] - \sum_{i=l+1}^{m} \beta_{i,l} n_i(t) n_l(t). \quad \text{[A-12]}$$

Combining the last three terms in Eq. [A-12] results in the classical discrete form of the coagulation equation

$$\frac{dn_l(t)}{dt} = \frac{1}{2}\sum_{i=1}^{l-1} \beta_{i,l-i} n_i(t) n_{l-i}(t) - n_l \sum_{i=1}^{m} \beta_{i,l} n_i(t) \quad \text{[A-13]}$$

where the first term on the right-hand side of Eq. [A-13] is evaluated only for $l > 1$.

APPENDIX B. EXACT EXPRESSIONS FOR BROWNIAN SECTIONAL COAGULATION COEFFICIENTS

The coagulation coefficient for particles in the continuum regime undergoing Brownian coagulation is given by (12),

$$\beta = \frac{2kT}{3\eta}\left[2 + \frac{D_i}{D_j} + \frac{D_j}{D_i} + A\left(\frac{1}{D_i} + \frac{1}{D_j} + \frac{D_i}{D_j^2} + \frac{D_j}{D_i^2}\right)\right] \quad \text{[B-1]}$$

where k is Boltzmann's constant, T is the absolute temperature, η is the viscosity of the medium, D_i and D_j are the diameters of the coagulating particles, and A is a first-order slip correction factor, approximately equal to 2.51λ, where λ is the mean free path of the medium.

For $f(v) = v$, ${}^4\bar{\beta}_{i,l}$ for Brownian coagulation is given by,

$$\begin{aligned} {}^4\bar{\beta}_{i,l} = \frac{\pi^{2-\gamma} 6^{\gamma-1} kT}{\alpha\eta(v_i - v_{i-1})(v_l - v_{l-1})} \Bigg\{ & \frac{2D^{3-3\gamma}\tilde{D}^3}{3(3-3\gamma)} + \frac{D^{4-3\gamma}\tilde{D}^2}{2(4-3\gamma)} + \frac{D^{2-3\gamma}\tilde{D}^4}{4(2-3\gamma)} \\ & + A\left[\frac{D^{2-3\gamma}\tilde{D}^3}{3(2-3\gamma)} + \frac{D^{3-3\gamma}\tilde{D}^2}{2(3-3\gamma)} + \frac{D^{4-3\gamma}\tilde{D}}{4-3\gamma} + \frac{D^{1-3\gamma}\tilde{D}^4}{4(1-3\gamma)}\right]\Bigg\} \Bigg|_{\tilde{D}=D_{l-1}}^{D_l} \Bigg|_{D=D_{i-1}}^{D_i} \end{aligned} \quad \text{[B-2]}$$

where D_i is the diameter of a particle of volume v_i and

$$\Bigg|_{\tilde{D}=D_{l-1}}^{D_l} \Bigg|_{D=D_{i-1}}^{D_i} \quad \text{[B-3]}$$

indicates that the expression is to be evaluated at $[D = D_i, \tilde{D} = D_l]$, minus that at $[D = D_i, \tilde{D} = D_{l-1}]$, minus that at $[D = D_{i-1}, \tilde{D} = D_l]$, and finally plus that at $[D = D_{i-1}, \tilde{D} = D_{l-1}]$. Factors of the form D^z/z are replaced by $\ln(D)$ if γ is such that $z = 0$.

For $f(v) = v$, $\alpha = 1$ and $\gamma = 0$, ${}^1\bar{\beta}_{i,l-1,l}$ for Brownian coagulation, $i < l - 1$, and the geometric constraint is given by,

$$
\begin{aligned}
{}^1\bar{\beta}_{i,l-1,l} = {} & \frac{\pi^2 kT}{6\eta(v_i - v_{i-1})(v_{l-1} - v_{l-2})}\Bigg\{-\frac{D^{11}}{396D_{l-1}^5} + D^{10}\left[\frac{1}{180D_{l-1}^4} + \frac{A}{120D_{l-1}^5}\right] + \frac{D^9A}{162D_{l-1}^4} \\
& - \frac{D^8}{144D_{l-1}^2} + \frac{D^7}{21}\left[\frac{5A}{6D_{l-1}^2} + \frac{1}{D_{l-1}}\right] + \frac{D^6}{18}\left[2 + \frac{A}{D_{l-1}}\right] + \frac{D^5}{15}(D_{l-1} + A) \\
& + \frac{D^4AD_{l-1}}{12} + \sum_{p=3}^{\infty} \frac{D^{3p}}{3^p p!D_{l-1}^{3p}}\Bigg(\Bigg[\frac{3AD^4D_{l-1}}{3p+4} + \frac{ADD_{l-1}^4}{3p+1} - \frac{D^5D_{l-1}}{3p+5} \\
& + \frac{D^2D_{l-1}^4}{3p+2}\Bigg]\left[\frac{\prod_{j=0}^{p-2}(2+3j)}{4}\right] + \left[\frac{D^4D_{l-1}^2}{3p+4} + \frac{AD^3D_{l-1}^2}{3p+3}\right]\left[\prod_{j=0}^{p-3}(4+3j)\right]\Bigg)\Bigg\}\Bigg|_{D_{i-1}}^{D_i}. \qquad \text{[B-4]}
\end{aligned}
$$

For $f(v)$ given by Eq. [20], ${}^4\bar{\beta}_{i,l}$ for Brownian coagulation, $\alpha = 1$ and $\gamma = 0$ is given by,

$$
\begin{aligned}
{}^4\bar{\beta}_{i,l} = {} & \frac{2kT}{3\eta(x_i - x_{i-1})(x_l - x_{l-1})} \\
& \times \Bigg\{2x\tilde{x} - \frac{2\cosh[\psi(\tilde{x} - x)]}{\psi^2} \\
& - \frac{A}{\psi 1 \mu\mathrm{m}}\Bigg[\tilde{x}e^{-\psi x} + xe^{-\psi\tilde{x}} \\
& + \frac{e^{\psi(x-2\tilde{x})} + e^{\psi(\tilde{x}-2x)}}{2\psi}\Bigg]\Bigg\}\Bigg|_{\tilde{x}=x_{l-1}}^{x_l}\Bigg|_{x=x_{i-1}}^{x_i} \qquad \text{[B-5]}
\end{aligned}
$$

where $\psi = \ln 10$.

Although, in general, one may be required to evaluate the inter- and intrasectional coagulation coefficients numerically, the computational effort can be significantly reduced if the inner integration can be evaluated analytically. One can of course obtain additional analytical expressions for sectional coefficients. However, the expressions given in this appendix were presented mainly to demonstrate that for realistic coagulation coefficients some sectional coefficients can be determined analytically.

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