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New analytical TEMOM solutions for a class of collision kernels in the theory of Brownian coagulation

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HIGHLIGHTS

- New class of analytical moment solutions of the Smoluchowski equation is found.
- The relative rates of solutions have asymptotically universal behavior.
- The results for a constant collision kernel are close to that for diffusion kernel.

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ABSTRACT

New analytical solutions in the theory of the Brownian coagulation with a wide class of collision kernels have been found with using the Taylor-series expansion method of moments (TEMOM). It has been shown at different power exponents in the collision kernels from this class and at arbitrary initial conditions that the relative rates of changing zeroth and second moments of the particle volume distribution have the same long time behavior with power exponent −1, while the dimensionless particle moment related to the geometric standard deviation tends to the constant value which equals 2. The power exponent in the collision kernel in the class studied affects the time of approaching the self-preserving distribution, the smaller the value of the index, the longer time. It has also been shown that constant collision kernel gives for the moments in the Brownian coagulation the results which are very close to that in the continuum regime.

1. Introduction

Equations of population balance (PBE) are general mathematical framework of statistical mechanics for modeling reversible and irreversible aggregation kinetics in different systems. They are used for aging aerosol dispersions in the gas atmosphere [1–3], for colloidal and polymer dispersions in solutions [4–6], and micellar systems [7,8]. In terms of time-dependent distribution of particles in sizes, i.e., one-particle density depending on particle size and time, the continuous form of PBE for irreversible aggregation is called the integro-differential Smoluchowski equation. It takes the form [1–3]

$$\frac{\partial n(\upsilon,t)}{\partial t}=\frac{1}{2}\int_0^{\upsilon}\beta(\upsilon_1,\upsilon-\upsilon_1)n(\upsilon_1,t)n(\upsilon-\upsilon_1,t)\mathrm{d}\upsilon_1-n(\upsilon,t)\int_0^{\infty}\beta(\upsilon_1,\upsilon)n(\upsilon_1,t)\mathrm{d}\upsilon_1 \tag{1}$$

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where $n(\upsilon, t)\mathrm{d}\upsilon$ is the number of particles at time t per unit volume of the system with particle volume varying from υ to $\upsilon + \mathrm{d}\upsilon$, the kernel $\beta(\upsilon_1, \upsilon)$ is the collision frequency function of coagulation which describes the frequency of coagulation of particles with volumes υ and υ_1.

In view of the nonlinear integro-differential structure of Eq. (1), only a limited number of known analytical and asymptotic solutions exist for simple model coagulation kernels β [9–12]. Among the different coagulation kernels, the collision frequency function for the continuum diffusion (or hydrodynamic) regime in the form

$$\beta(\upsilon, \upsilon_1) = (\upsilon^{1/3} + \upsilon_1^{1/3})(\upsilon^{-1/3} + \upsilon_1^{-1/3}) \tag{2}$$

has wide applications and a particular significance in practice not only in describing aerosol agglomeration, but also in the theory of Brownian coagulation in colloidal solutions, in flocculation and other related processes. In addition, the constant collision frequency also indicates itself as a convenient model for many aggregation processes.

Because of the relative simplicity of implementation and low computational cost, the different methods for the moments of the time-dependent distribution of particles in sizes have been used extensively to solve various kinetic problems, and now the moment methods became a powerful theoretical tool for microphysical investigation of coagulation processes [13]. Recently, Yu et al. [14] have presented a new moment-based numerical approach to solve the coagulation equation (1). This approach was named as the Taylor-series Expansion Method Of Moments (TEMOM). In the TEMOM method, the set of the moment equations for the distribution of particles in their volumes is closed with using the Taylor-series expansion of collision kernels. Through constructing a closed set of three first-order ordinary differential equations, the most important moments for describing the particle dynamics, namely, the particle number density, total particle volume and geometric standard deviation for particle volume, can be obtained. This approach makes no prior assumption on the shape of the particle volume distribution; therefore, the limitation inherent in the lognormal distribution theory [13] automatically disappears. Several studies [15–17] have recently demonstrated that TEMOM is a promising method to approximate, with a high degree of physical accuracy and computational efficiency, a solution of the full aerosol population balance equation (1). Some similarities with this method can also be found in the moment analysis of micellization kinetics for short and lengthy micelles presented in Ref. [18].

Since the PBE with a homogeneous kernel is invariant under a group of similarity transformations, it admits self-similar or scaling solution. Friedlander's theory of self-preserving spectra [1,19,20] gave a satisfactory explanation of the experimental observations of Brownian coagulation in the hydrodynamic and free molecular regimes for the collision frequencies. Using the TEMOM method, Xie & Wang [21] and Xie & He [22] presented an elegant asymptotic solution and analytical solution of PBE for Brownian coagulation in the free molecular and continuum regimes for the collision frequencies. Xie [23] also have analyzed the asymptotic behavior in the TEMOM method over the entire particle size range at different Knudsen numbers. These results show that all moments of the distribution function $n(\upsilon, t)$ at large times depend explicitly on time and the first moment (i.e., total volume of particles).

In the present study, we will develop our previous work [20,21] and obtain a class of analytical solutions for the particle population balance equation with the collision kernels modeled as

$$\beta = (\upsilon^{a} + \upsilon_1^{a})(\upsilon^{-a} + \upsilon_1^{-a}) \tag{3}$$

where the exponent a ($a \geq 0$) is a non-negative constant. If $a = 0$, the collision kernel is constant. In the case of $a = 1/3$, Eq. (3) is reduced to Eq. (2) for the collision kernel for Brownian coagulation in the continuum diffusion regime. Under assumption of stationary collision rates, for arbitrary particle agglomerate formation and restructuring, the exponent a can be considered as the inverse function of fractal dimension D_f, i.e., $a = 1/D_f$. The value of D_f depends on the details of the aggregation process; for chain-like structures, $D_f \to 1$, while for compact aggregates, $D_f \to 3$.

In coagulation of particles, the size of the particles may be initially small in the free molecule regime, however the particle volume will grow due to coagulation, and the collision frequency will change from that for the free molecular regime via the transition regime to the collision frequency for near continuum and continuum regime. Correspondingly, the asymptotic behavior of the PBE solution will gradually tend to that in the continuum regime [21–23]. Therefore, the characteristics of particle agglomeration in the continuum regime are of great importance for understanding the coagulation mechanism. However, a complicated mathematical form of the Brownian coagulation kernel for the continuum regime does not allow making an analysis of the PBE on an analytical level. As follows from Eq. (3) and the idea of the TEMOM method, the difference between two sets of solutions for $a = 0$ and $a = 1/3$ can be small. Below we will show that this is true, and the description of Brownian coagulation in the continuum regime may be simplified by using a constant collision kernel in some cases.

2. The moment equations

The Taylor series expansion method of moments (TEMOM) is designed to solve the particle population balance equation for time-dependent distribution $n(\upsilon, t)$ of particles in their volumes υ. The kth moment M_k of the particle distribution is defined as

$$M_k(t) = \int_0^\infty \upsilon^k n(\upsilon, t)\mathrm{d}\upsilon. \tag{4}$$