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Asymptotic behavior of the Taylor-expansion method of moments for solving a coagulation equation for Brownian particles

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ABSTRACT

The evolution equations of moments for the Brownian coagulation of nanoparticles in both continuum and free molecule regimes are analytically studied. These equations are derived using a Taylor-expansion technique. The self-preserving size distribution is investigated using a newly defined dimensionless parameter, and the asymptotic values for this parameter are theoretically determined. The dimensionless time required for an initial size distribution to achieve self-preservation is also derived in both regimes. Once the size distribution becomes self-preserving, the time evolution of the zeroth and second moments can be theoretically obtained, and it is found that the second moment varies linearly with time in the continuum regime. Equivalent equations, rather than the original ones from which they are derived, can be employed to improve the accuracy of the results and reduce the computational cost for Brownian coagulation in the continuum regime as well as the free molecule regime.

1. Introduction

The Brownian coagulation of nanoparticles is of great importance in many fields, such as atmospheric science and combustion technology, because it can significantly influence the size distribution of the nanoparticles. Many properties of nanoparticles, such as light scattering and toxicity as well as physical processes including diffusion and condensation, depend strongly on their size distribution. By solving the particle general dynamic equation (PGDE), the evolution of particle size distribution can be traced (Müller, 1928). However, only a limited number of known analytical solutions can be obtained because of the complexity of the mathematical models and the difficulty of solving the nonlinear integro-differential PGDE. Therefore, several numerical techniques, including the method of moments (Lee, 1983; McGraw, 1997; Pratsinis, 1988; Yu, Lin, & Chan, 2008), the sectional method (Gelbard & Seinfeld, 1980; Gelbard, Tambour, & Seinfeld, 1980), and the stochastic particle method (Morgan, Wells, Goodson, Kraft, & Wagner, 2006), have been proposed to obtain approximate solutions. The method of moments is superior to other methods in terms of its high efficiency.

The method of moments, which typically solves the first three moments of the particle volume distribution, is relatively simple to implement, and has become a useful tool for investigating representative properties of particle systems, such as the particle concentration, mean size, and polydispersity. The conventional method of moments has the disadvantage that the particle size distribution must be specified in advance for the closure of the evolution equations. McGraw (1997) developed the quadrature method of moments (QMOM), which overcomes this problem by approximating the integral moment with a Gaussian quadrature. However, the weights and abscissas of the quadrature approximation must be obtained using certain algorithms, such as the product-difference algorithm (Gordon, 1968; Press & Teukolsky, 1990). This greatly increases the computational cost in comparison with other methods of moments, especially when computational fluid dynamics is considered.

By assuming to be a time-dependent log-normal function, the particle size distribution, median particle volume and geometric standard deviation based on particle radius has been analyzed for Brownian coagulation in the continuum regime (Lee, 1983; Lee, Lee, & Han, 1997), free molecule regime (Lee, Chen, & Gieseke, 1984; Lee, Curtis, & Chen, 1990), and in the entire regime (Otto, Fissan, Park, & Lee, 1999; Park, Lee, Otto, & Fissan, 1999). They also confirmed that there exists an asymptotic distribution that preserves a fixed form. The results were compared with the self-preserving

Abbreviations: ODEs, ordinary differential equations; PGDE, particle general dynamic equation; QMOM, quadrature method of moments; SPSD, self-preserving size distribution; TEMOM, Taylor-expansion method of moments.

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size distribution (SPSD) obtained by similarity theory (Friedlander & Wang 1966; Friedlander, 2000).

To avoid the disadvantage of specifying the particle size distribution in advance and reduce the computational cost, Yu et al. (2008) put forward the Taylor-expansion method of moments (TEMOM), which behaved well in both the free molecule and continuum regimes. Yu, Lin, Jin, and Jiang (2011) further extended TEMOM to the entire size regime by means of harmonic mean approximation and Dahneke approximation. The time-dependent geometric standard deviation was also calculated numerically for the case where the particle size satisfies a log-normal distribution. In the present study, we mainly focused on the asymptotic behavior of TEMOM, i.e., the numerical results after a sufficiently long time. A newly defined parameter was used to investigate the self-preserving property of Brownian particles in the continuum regime and the free molecule regime. The asymptotic values of this parameter were determined analytically using the original TEMOM equations in both regimes. Once the particle size distribution achieved self-preservation, the time evolutions of the zeroth moment and second moment could be derived analytically. These asymptotic expressions were then compared with those given by log-normal preserving theory and similarity theory. The time required to reach SPSD is also determined theoretically and expressed as a function of the initial size distribution. The approach to solving the sets of ordinary differential equations (ODEs) derived via TEMOM is improved by simplifying the ODEs. A linear evolution of the second-order moment in the continuum regime can be observed as long as the size distribution becomes self-preserving.

2. Theory of TEMOM

The PGDE for the Brownian coagulation of nanoparticles can be written as (Müller, 1928):

$$\frac{\partial n(v,t)}{\partial t} = \frac{1}{2}\int_0^v \beta(v-v_1,\, v_1)n(v-v_1,\, t)n(v_1,\, t)dv_1 - n(v,\, t)\int_0^\infty \beta(v,\, v_1)n(v_1,\, t)dv_1, \tag{1}$$

where v and v_1 are the particle volumes, $n(v,\, t)$ is the particle size distribution, and $\beta(v,\, v_1)$ is the collision kernel for two particles of volumes v and v_1. Multiplying Eq. (1) by v^k and integrating over v, the equations for the moments of the particle size distribution are obtained (Barrett & Webb, 1998):

$$\frac{dm_k}{dt} = \frac{1}{2}\int_0^\infty \int_0^\infty \left[(v_1+v_2)^k - {v_1}^k - {v_2}^k\right] \times \beta(v_1,\, v_2)n(v_1,\, t)n(v_2,\, t)dv_1dv_2, \tag{2}$$

where the moments m_k are defined by

$$m_k = \int_0^\infty v^k n(v,\, t)dv. \tag{3}$$

Yu et al. used TEMOM to solve this problem by disposing of the collision kernel and the fractional moments in a particular way (Yu et al., 2008; Yu & Lin, 2009). The evolution equations of moments for the Brownian coagulation of nanoparticles derived using a 3rd-order TEMOM can be expressed as, for the free molecule regime,

$$\frac{dm_0}{dt} = \frac{\sqrt{2}K_{\mathrm{fm}}}{5184}\frac{m_0^{11/6}(65m_0^2m_2^2 - 1210m_0m_1^2m_2 - 9223m_1^4)}{m_1^{23/6}}, \tag{4.1}$$

$$\frac{dm_1}{dt} = 0, \tag{4.2}$$

$$\frac{dm_2}{dt} = -\frac{\sqrt{2}K_{\mathrm{fm}}}{2592}\frac{701m_0^2m_2^2 - 4210m_0m_1^2m_2 - 6859m_1^4}{m_0^{1/6}m_1^{11/6}}, \tag{4.3}$$

for the continuum regime,

$$\frac{dm_0}{dt} = \frac{K_C}{81}\frac{m_0^2(2m_0^2m_2^2 - 13m_0m_1^2m_2 - 151m_1^4)}{m_1^4}, \tag{5.1}$$

$$\frac{dm_1}{dt} = 0, \tag{5.2}$$

$$\frac{dm_2}{dt} = -\frac{2K_C}{81}\frac{2m_0^2m_2^2 - 13m_0m_1^2m_2 - 151m_1^4}{m_1^2}, \tag{5.3}$$

where $K_{\mathrm{fm}} = (3/4\pi)^{1/6}(6k_BT/\rho)^{1/2}$ and $K_C = 2k_BT/3\mu$ are the coagulation coefficients for the free molecule regime and continuum regime, respectively, k_B is the Boltzmann constant, T is the absolute gas temperature, ρ is the mass density of the particles, and μ is the gas viscosity. These systems of ODEs are solved using a 4th-order Runge–Kutta method with a fixed time step.

3. Asymptotic behavior of TEMOM

Most studies have shown that the SPSD exists (Swift & Friedlander, 1964; Hidy, 1965; Friedlander & Wang 1966; Lai, Friedlan, Pich, & Hidy, 1972), and it has become an important tool for exploring particle coagulation mechanisms. Friedlander and Wang (1966) studied the theoretical coagulation equation in the continuum regime by means of a similarity transformation, and Lai et al. (1972) used the same transformation to study the coagulation equation in the free molecule regime. This transformation leads to an ordinary integro-differential equation for both the free molecule and continuum regimes, and numerical solutions for these equations can be obtained by a finite-difference method. The transformation introduced by Swift and Friedlander (1964) is given by

$$n(v,\, t) = \frac{m_0^2}{m_1}\psi(\eta), \tag{6}$$

$$\eta = \frac{m_0}{m_1}v, \tag{7}$$

where m_0 and m_1 are the zeroth and first moments of the particle size distribution, $\psi(\eta)$ is the reduced size distribution, and η is the dimensionless volume. It is assumed that the reduced size distribution $\psi(\eta)$ is independent of time and approaches a self-preserving form after a sufficiently long time. For a self-preserving distribution, the following equation can be derived

$$m_2 = \frac{m_1^2}{m_0}\int_0^\infty \eta^2\psi(\eta)d\eta. \tag{8}$$

We can define a dimensionless parameter using the first three moments, that is,

$$\theta = \frac{m_0m_2}{m_1^2}, \tag{9}$$

which is constant for a self-preserving distribution because it equals the integral in Eq. (8), which is independent of time. This parameter will be used to investigate the SPSD for Brownian coagulation. It can be related to the dimensionless geometric standard deviation σ_g used by Lee (1983) and Yu et al. (2008) if the particle size distribution is assumed to be log-normal. The relationship between these two parameters is given by

$$\ln^2\sigma_g = \frac{1}{9}\ln\theta. \tag{10}$$