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An approximate theoretical solution to particle coagulation and gelation using a method of moments

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ABSTRACT

An approximate scheme that permits a much simplified application of method of moments to the study of aerosol coagulation and gelation processes has been proposed and verified in this work. The central idea underlying the scheme is to express a fractional moment in terms of its adjacent integer moments. In this manner the moment equations are then decoupled, and can be solved separately and analytically. The crucial rules for approximating fractional moments are proposed. A method of moments using the new scheme is applied to the study of aerosol coagulation characterized by various collision kernels, including Brownian kernels in the free-molecular and continuum regime and parametric gelling kernel. The computational accuracy of the proposed scheme is validated with a sectional model. The simulational results are extensively compared with previously published results.

1. Introduction

The study of coagulation and/or coalescence of particles has long been a topic of paramount importance in a wide variety of aerosol-related disciplines, including material synthesis, combustion, polymerization, contamination control. These mechanisms play a significant role in many aerosol processes by profoundly affecting the growth characteristics, the morphology, as well as the size distribution of a particle system. Particle coagulation is in general considered as a time-dependent process governed by the following population balance equation (PBE), the Smoluchowski's equation (Friedlander, 1997; Fuchs, 1989),

$$\frac{\partial n_p(v,t)}{\partial t} = \frac{1}{2}\int_0^v K(v-u,u)n_p(u,t)n_p(v-u,t)du, -n_p(v,t)\int_0^\infty K(v,u)n_p(u,t)du \tag{1}$$

where $n_p(v,t)$ is in general the number concentration of particles of volume v at time t, $K(u,v)$ is the collision kernel for describing the frequency in which two particles of volume u and v collide with each other.

Eq. (1) is a non-linear integro-differential equation, which is in general not analytically intractable except for some specific, simple kernels, such as constant kernel. For most realistic kernels, finding a solution to above PBE is non-trivial and considerable effort has been expended in developing various useful methods for this purpose. Based on different disciplines these methods can broadly be categorized into deterministic methods and stochastic methods; the former include methods of moments (Brown, Kauppinen, Jokiniemi, Rubin, & Biswas, 2006; McGraw, 1997; Terry, McGraw, & Rangel, 2001; Yu, Lin, & Chan, 2008), sectional methods (Jeong & Choi, 2001; Landgrebe & Pratsinis, 1990; Mitrakos, Hinis, & Housiadas, 2007; Pyykönen & Jokiniemi, 2000; Wu & Biswas, 1998), uni-model/bi-model (Jenong & Choi, 2003; Kruis, Kusters, Pratsinis, & Scarlett, 1993) based on solving a set of differential equations analytically or numerically; while the latter involve primarily Monte Carlo methods (Garcia, Broeck, Serneels, & Aertsens, 1987; Kruis, Maisels, & Fissan, 2000; Lee & Matsoukas, 2000; Zhao, Kruis, & Zheng, 2009). Among all

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these schemes, method of moments has proved to be mathematically rigorous and numerically economical. A method of moments is able to offer a simple yet effective means for the description of dynamic behaviors of a particle ensemble by tracking the time rate of change of moments of the quantities one considers. Such quantities can be particle volume, particle charge, etc. The nth moment of particle ensemble, M_n, in terms of particle volume is in general defined by

$$M_n = \int_0^\infty v^n n(v, t) dv. \tag{2}$$

Multiplying both sides of Eq. (1) with v^n, integrating over all the particle sizes and using Eq. (2), one obtains (Williams & Loyalka, 1991)

$$\dot{M}_n = \frac{1}{2} \int_0^\infty du \int_0^\infty f(u, v, n) K(u, v) n_p(v, t) n_p(u, t) dv, \tag{3}$$

where function $f(u, v, n)$ is given by $f(u, v, n) = (u + v)^{nn} - u^n - v^n$. It is clear that function $f(u, v, n)$ respectively outputs -1, 0 and $2uv$ for the first three integer moments.

At this point one can derive a set of ordinary differential equations (ODE) from Eq. (3). Through solving these equations, one can readily obtain information about the interesting properties about the particle ensemble without tracking the entire particle size spectrum, which may include hundreds or thousands size bins. This feature renders a moment model almost computational instantaneous, especially compared with its time-consuming counterparts, e.g. a Monte Carlo method. Moreover, under certain circumstances a method of moments can provide a relatively accurate description of evolution of the particle system by solving Eq. (1) analytically. Methods of moments face also several shortcomings. One such shortcoming is that the implementation of a moment model could be extremely tedious in some cases; for example, the resultant moment expressions formulated in a bipolarly charging process of ultrafine aerosol particles are quite complex (Park, Lee, Shimada, & Okuyama, 2005). In addition, although many moment models do not require assumptions on the functional form (e.g. a log-normal model) of the particle size distribution, few such models (Lee, Chen, & Gieseke, 1984) are still relying on a prior knowledge of the size distribution.

When applying method of moments one often needs to deal with fractional moments, whose appearance is due to the physical derivation of the original collision kernels. Several schemes are now available for handling this issue. One feasible scheme is to use an auxiliary equation, which is derived based on a priori assumption of the particle size distribution. With the help of this equation one can evaluate an arbitrary fractional moment (Lee et al., 1984; Park et al., 2005; Peterson, Gelbard, & Seinfeld, 1978). Another method is to express a fractional moment in terms of a function with respect to several integer or non-integer moments using a Taylor-series expansion technique (Yu, Liu, Lin, & Seipenbusch, 2015; Yu et al., 2008). The most straightforward scheme is perhaps to express a fractional moment in terms of several integer moments using some interpolation techniques, such as Lagrange polynomials (Estrada & Cuzzi, 2008; Frenklach, 2002). In the framework of such a scheme a fractional moment M_p (p is a non-integer order) in the normalized form, $M'_p = M_p/M_p(0)$(where $M_p(0)$ is the initial value of M_p), can be expressed by$M'_p(t) \cong \prod_{j=k}^{k+n} [M'_j(t)]^{L_j^n(p)}$ with n being the maximum moment order and exponent $L_j^n(p)$ a Lagrange interpolation with respect to p. The interpolation scheme is straightforward which does not involve any priori assumptions. However, by simply expressing a fractional M_p as a function of the whole-order integer moments, one may encounter relatively complex expressions for fractional moments, which further give rise to a set of coupled and complicated ODEs that can only be solved numerically. This is particularly true for the case when the collision kernel is parametrically expressed.

In this work we devise an approximate yet effective scheme, for dealing with those fractional moments in hope of providing a simple method of moments for analyzing various aerosol coagulation processes. The new scheme is based largely upon the idea of expressing a fractional moment only in terms of its adjacent integer moments, but not the whole-order moments as above. The concept of adjacent moments with respect to a fractional moment will be discussed in the next section. We propose the related rules for expressing a fractional moment in terms of the relevant integer moments. To verify the proposed scheme, we further apply a method of moments using the new scheme to the study of coagulation processes characterized by various collision kernels.

2. Methodology

The crucial idea underlying the present scheme is elucidated by a particular example of case study, namely applying a moment method to study aerosol coagulation governed by Brownian kernel in the continuum regime. The kernel in this regime has the general form (Mountain, Mulholland, & Baum, 1986)

$$K(u, v) = K_0(u^\alpha + v^\alpha)(u^{-\alpha} + v^{-\alpha}), \quad 0 \le \alpha \le 1, \tag{4}$$

where K_0 is the collision coefficient, α is the exponent. Typically, α take the following values: (1) $\alpha = 0$; in this case K reduces to constant kernel; (2) $\alpha = 1/3$; K turns out to be Brownian kernel in the continuum regime for spherical particles; (3) $\alpha = D_f$ where D_f is the fractal dimension; kernel is now applicable to modeling coagulation of particle clusters due to the Brownian motion.

One can combine Eq. (4) with Eq. (3) and obtain the following moment equations

$$\begin{cases} \dot{M}_0 = -K_0(M_0^2 + M_\alpha M_{-\alpha}) \\ \dot{M}_1 = 0 \\ \dot{M}_2 = 2K_0(M_1^2 + M_{1+\alpha} M_{1-\alpha}) \end{cases}. \tag{5}$$