Journal of Aerosol Science 67 (2014) 28–37

Contents lists available at ScienceDirect

Journal of Aerosol Science

journal homepage: www.elsevier.com/locate/jaerosci

Direct expansion method of moments for nanoparticle Brownian coagulation in the entire size regime

Zhongli Chen [a], Jianzhong Lin [a,b,*], Mingzhou Yu [b,c]

[a] School of Aeronautics and Astronautics, Zhejiang University, Hangzhou 310027, China
[b] China Jiliang University, Hangzhou 310018, China
[c] Karlsruhe Institute of Technology, Institute for Mechanical Process Engineering and Mechanisms, Karlsruhe, Germany

ARTICLE INFO

Article history:
Received 22 April 2013
Received in revised form
11 August 2013
Accepted 20 August 2013
Available online 3 October 2013

Keywords:
Brownian particles
Coagulation
Entire size regime
Method of moments
Accuracy

ABSTRACT

The direct expansion method of moments for nanoparticle Brownian coagulation is investigated in the entire size regime. The exact Dahneke's formula is used as the coagulation kernel. After comparing the results predicted by the direct expansion method of moments with those provided by the quadrature method of moments, the direct expansion method is proved to be qualified for predicting the time evolution of the lower order moments such as the zeroth and second moments. For relatively small initial geometric standard deviation, the results predicted by the direction expansion method of moments are more accurate than those provided by the quadrature method of moments. The partial derivatives of the coagulation kernel that appear in the direction expansion method of moments are calculated numerically due to the complicated form of the selected kernel, and the computational time can be reduced by means of parallel computing.

1. Introduction

Nanoparticle Brownian coagulation is a process whereby individual nanoparticles collide with one another and stick together to form larger particles due to their relative Brownian motion. The net result of nanoparticle coagulation is a decrease in number concentration as well as an increase in particle size. The evolution of nanoparticle size distribution can be traced by means of solving the particle general dynamic equation (PGDE) analytically or numerically. Only a limited number of analytical solutions of the PGDE can be found because of its nonlinear integro-differential nature. As a result, several numerical methods have been proposed and developed to obtain the approximate solutions, such as the method of moments (MOM) (Lee, 1983; Frenklach & Harris, 1987; Pratsinis, 1988; McGraw, 1997; Yu et al., 2008) and the sectional method (SM) (Gelbard & Seinfeld, 1980; Gelbard et al., 1980; Wu & Flagan, 1988; Landgrebe & Pratsinis, 1990). Different methods are used in different fields to meet particular practical requirement according to their different advantages and disadvantages in accuracy and efficiency. The method of moments is prior to the sectional method in efficiency while the sectional method is more accurate than the method of moments.

The method of moments, which typically solves the first three moments of particle volume distribution, is computationally efficient and has become a useful tool for investigating the evolution of the representative properties of

* Corresponding author at: School of Aeronautics and Astronautics, Zhejiang University, Hangzhou 310027, China. Tel.: +86 571 86836009; fax: +86 571 86914401.
E-mail address: mecjzlin@public.zju.edu.cn (J. Lin).

0021-8502/$ - see front matter © 2013 Published by Elsevier Ltd.
http://dx.doi.org/10.1016/j.jaerosci.2013.08.011

nanoparticle system such as particle concentration and mean volume. Conventionally, the closure of moment evolution equations is achieved by specifying the shape of the particle size distribution in advance (Lee, 1983; Lee et al., 1984; Pratsinis, 1988). By assuming the particle size distribution to be a time-dependent log-normal function, Lee (1983) first analytically studied the particle size distribution and geometric standard deviation for Brownian coagulation in the continuum regime. The same technique was used to investigate Brownian coagulation in the free molecular regime (Lee et al., 1984) and the entire size regime (Otto et al., 1999; Park et al., 1999). To get rid of the restriction of specifying particle size distribution in advance, McGraw (1997) proposed the quadrature method of moments (QMOM) by using an n-point Gaussian quadrature to approximate the integral terms that appear in the moment evolution equations. The QMOM has been proved to be valid and applied to any form of coagulation kernels. However, the weights and abscissas of the quadrature approximation must be calculated by means of certain algorithms such as product-difference algorithm (Gordon, 1968; Press & Teukolsky, 1990), long quotient-modified difference algorithm (Sack & Donovan, 1971) and Golub–Welsch algorithm (Golub & Welsch, 1969), which makes the QMOM a computationally expensive method in comparison with other methods of moments. To avoid this disadvantage, Yu et al. (2008) put forward a new numerical method named Taylor-expansion method of moments (TEMOM) for Brownian coagulation in both free molecular and continuum regimes, and it has been further extended to the entire size regime (Yu et al., 2011). However, the moment transfer for the TEMOM could not be accomplished when the coagulation kernel is sufficiently complex, e.g., Fuchs' semi-empirical coagulation kernel for Brownian coagulation in the transition regime (Fuchs, 1964). In this article, therefore, we take advantage of a newly proposed method of moments, namely the direct expansion method of moments (DEMM), which is based on the TEMOM with the basic idea of closing the moment evolution equations by means of Taylor-series expansion technique. The DEMM makes it possible to use the fractional order moments to improve the accuracy of the results, and has the potential to deal with complex coagulation kernels.

In the present study, we focus on the Brownian coagulation in the entire size regime using the DEMM with one selected coagulation kernel and compare the DEMM with QMOM both in accuracy and efficiency under the same computational condition. Meanwhile, the sectional method is used as a reference for validating other methods due to its high accuracy.

2. Theory

There are two ways to describe the coagulation process. The first one is put forward by Smoluchowski (1917), who developed expressions for discrete particle size distribution. The second one, which is used in the present study, assumes that the particle size distribution is continuous. The particle size distribution of a nanoparticle system undergoing coagulation is governed by a nonlinear integro-differential equation in case that a continuous particle size distribution is utilized (Müller, 1928; Friedlander, 2000), i.e.,

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

where v and v_1 are the particle volumes, $n(v,t)$ is the particle size distribution and $\beta(v,v_1)$ is the coagulation kernel for two particles of volumes v and v_1.

The nanoparticle dynamics depends upon the Knudsen number Kn ($Kn=\lambda/\alpha$, where λ is the molecular mean free path in the gas and a is the radius of nanoparticle). There are two limiting regimes corresponding to large and small values of Kn for which the theories are well characterized, namely the near-continuum regime ($Kn<1$) and free molecular regime ($Kn>50$). The coagulation kernel for the near-continuum regime can be expressed as

$$\beta_{co}(v_1,v_2)=K_{co}(v_1^{1/3}+v_2^{1/3})\left(\frac{C(v_1)}{v_1^{1/3}}+\frac{C(v_2)}{v_2^{1/3}}\right), \tag{2}$$

where $K_{co}=2k_BT/3\mu$ is the coagulation coefficient for the continuum regime, k_B is the Boltzmann constant, T the absolute temperature, μ the gas viscosity and C is the Cunningham correction factor (Cunningham, 1910; Davies, 1945), which is given by

$$C=1+Kn[A_1+A_2\ \exp(-A_3/Kn)] \tag{3}$$

where A_1, A_2 and A_3 are constants.

The coagulation kernel for the free molecular regime is given by (Yu et al., 2009)

$$\beta_{fm}(v_1,v_2)=K_{fm}\left(\frac{1}{v_1}+\frac{1}{v_2}\right)^{1/2}(v_1^{1/3}+v_2^{1/3})^2 \tag{4}$$

where $K_{fm}=(3/4\pi)^{1/6}(6k_BT/\rho)^{1/2}$ is the coagulation coefficient for the free molecular regime and ρ is the mass density of the corresponding nanoparticle.

The transition regime is characterized by $1<Kn<50$ in which the coagulation kernel is described neither by the near-continuum theory nor the kinetic theory for the free molecular regime. Fuchs (1934) found a semi-empirical expression for the coagulation kernel by assuming that outside of the distance of an average mean free path of certain particles, the transport of particles is described by the continuum diffusion theory with Cunningham correction factor for slip, and inside this distance the particles move like in a vacuum. Dahneke (1983) also derived a solution of the coagulation kernel for the