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Review

Nanoparticle-laden flows via moment method: A review

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ABSTRACT

The study of nanoparticle-laden multiphase flow has received much attention due to its occurrence in a wide range of industrial and natural phenomena. Many of these flows are multi-dimensional multi-species systems involving strong mass, momentum and energy transfer between carrying phase and dispersed particle phase. The purpose of the present paper is to survey some advances on our researches in this field over the last 5 years. The research includes the closure for particle general dynamic equation; the fundamental interaction between particle dynamics and flow coherent structures; theoretical analysis on nanoparticle collision rate; and the application of theoretical works in some specific problems.

1. Introduction

The term "nanoparticle-laden multiphase flow" is defined here as aerocollodial or dispersed particulate systems in which the particle size is below 1 μm in diameter, which occurs in a wide range of industrial and natural phenomena such as nanoparticle synthesis, atmospheric sciences and air pollution, contamination control in the microelectronics and pharmaceuticals industries, and diesel particulate formation. Theoretically, the sizes of these particles span from free molecular size regime much less than Kolmogorov length scale to continuum range (Friedlander, 2000). These particles share energy with gas molecules and exhibit Brownian motion, and thus they have a thoroughly different mechanism and characterization of dispersion in turbulent flows from coarse particles and even fine particles (Chan et al., 2006). The study on this kind of multiphase system is required not only to grasp the interaction between the dispersed particles and the carrier phase, but also to obtain the fundamentals of internal processes including nucleation, chemical reaction, condensation, coagulation and breakage.

Relative to Kolmogorov length scale and time scale, there are generally very small size scale and inertial response time for nanoparticles. At this case, the particle Stokes number is sufficiently small implying the particles follow the local fluid motion precisely and their velocity slip can be neglected (Wang et al., 1998). Consequently, the study for the fluid and particle dynamics can be decoupled (Barthelmes et al., 2003). This disposition is greatly valid in most nanoparticle-laden multiphase systems, especially in the dilution condition where particle volume fraction is below 0.1% (Heine and Pratsinis, 2006, 2007). This method is also generally called one-way coupling method. Currently, some researchers still follow this method to investigate the nature of nanoparticle transport and dynamics in turbulent flows based on both the one-fluid approach (Chan et al., 2006; Johannessen et al., 2001) and the two-fluid approach (Garrick et al., 2006; Yu et al., 2008a,b; Marchisio and Fox, 2005). For nanoparticle-laden system, the two-fluid approach is prior to the one-fluid approach in that the evolution of particle dynamics, the heat and mass transfer between carried particulate phase and carrying phase, and the spectrum of particle size distribution can be more appropriately characterized in the framework of two-fluid approach. Therefore, one-way coupling method within a two-fluid framework may be the most useful solution for nanoparticle-laden systems.

In general studies on multiphase flows, two-fluid approach treats the suspension as two interacting continua, each phase having governing equation. Here, the governing equation for dispersed particles is also called convection–diffusion transport equation. However, only convection–diffusion transport equation cannot provide the information of some key parameters such as particle size, number concentration, and the spectrum of particle size distribution. In order to overcome this limit, the classic Smoluchowski mean-field theory (i.e., population balance modeling) is usually used (Smoluchowski, 1917). This theory defines particle concentration as a function of time and particle volume in a probability, and the relevant equation has natural superiority in coupling with computational fluid dynamic within an Eulerian framework. Thus, the combination of computational fluid dynamics and classic Smoluchowski mean-field theory provides a route to investigate

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the spatial temporal evolution of nanoparticles in turbulent flows. Nowadays, the study on nanoparticle-laden multiphase flow within the mean-field framework is still a hot and challenging issue due to unmanageable inter-particle collision or breakage rate (Heine and Pratsinis, 2006, 2007; Soos et al., 2008; Derevich, 2007; Duru et al., 2007), complicated closure problem for one and even multivariate population balance problems (Yu and Lin, 2009a,b; Kostoglou, 2007; Marchisio and Barresi, 2009), fractal structures (Schwager et al., 2008; Maricq, 2007) and unknown interaction between particles and carrying phase in dense or turbulent systems (Chun et al., 2005; Salazar et al., 2008; Brown et al., 2006; van der Hoef et al., 2008).

Over the past 5 years, we have done many investigations on nanoparticle-laden flows from the derivation of inter-particle collision rate to the application of our newly proposed Taylor-expansion moment method in specific problems. A brief review on these researches is presented in the followings.

2. The collision efficiency of spherical aerosol particles in the Brownian coagulation

For aerosols with particle diameter below 1000 nm, coagulation is the major mechanism leading to aerosol instability. In the Smoluchowski mean-field theory, it needs to give the coagulation rate in a probability, while the relevant study is still a challenging field.

Since Smoluchowski (1917) first proposed a collision rate for monodisperse aerosol particles, there have been a lot of researchers devoting to propose more accurate and appropriate models by concerning van der Waals forces, colloid force, non-continuum lubrication force, charged or non-spherical affect, and hydrodynamic particle interaction. However, the elastic force arising from particle deformation in the collision process was never taken into account in the above investigations.

In order to make sure whether the elastic force can be neglected relative to van der Waals force, Feng and Lin (2008) proposed a model representing interparticle collision rate by simultaneously considering both forces, shown in Fig. 1. As particles are assumed to follow Maxwell velocity distribution, Feng and Lin (2008) finally got the collision rate:

$$\alpha = \int_0^{v_{cr}} 4\pi\left(\frac{m}{2\pi kT}\right)^{3/2} e^{-(mv^2/2kT)}\, v^2\, dv \tag{1}$$

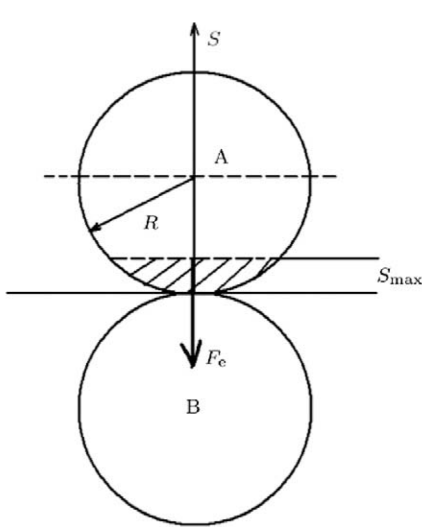

Fig. 1. Schematic diagram of the collision between two particles. R is the particle radius, while S_{max} is the maximum deformation.

where v_{cr} is critical velocity, k is Boltzmann constant, and T is temperature. Here, the critical velocity should be determined by Feng and Lin's analytical equations.

Using this equation, Feng and Lin (2008) investigated monodisperse aerosols with diameters ranging from 100 to 760 nm. They found the interparticle elastic deformation force cannot be neglected in the computation of particle Brownian coagulation. The newly proposed expression for collision rate is expected to be widely used in the following aerosol studies.

3. The closure for population balance equation with respect to Brownian coagulation

Although Smoluchowski established the Smoluchowski mean-field theory for aerosols and correspondingly proposed the Smoluchowski equation (population balance equation with respect to Brownian coagulation) about 90 years ago, the solution for Smoluchowski equation is still an open research field to date just because of the equation's non-linear characteristic. Generally, the Smoluchowski equation is more appropriately written by the following integro-differential form (Muller, 1928):

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

where $n(v, t)dv$ is the number of particles whose volume is between v and $v + dv$ at time t, and $\beta(v_1, v)$ is the collision kernel for two particles of volumes v and v_1.

The Smoluchowski equation is none other than Boltzmann's transport equation which has only a limited number of known analytical solutions due to its own non-linear integro-differential structure. Hence, an alternative method, the numerical technique, has to be used to obtain approximate solutions for it. However, the direct numerical calculations often become impractical, even with a modern super-computer, due to the requirement of large computational cost. In order to break the limit in computational cost, three prominent methods were usually used, i.e., the moment method (MM) (Hulbert and Katz, 1964; Frenklach, 2002; McGraw, 1997; Lee et al., 1984; Yu et al., 2008c), the sectional method (SM) (Gelbard and Seinfeld, 1980; Talukdar and Swihart, 2004; Kostoglou, 2007; Landgrebe and Pratsinis, 1990) and the stochastic particle method (SPM) (Wells and Kraft, 2005; Morgan et al., 2006). These methods have both advantages and disadvantages in accuracy and efficiency, and now they are used in different fields in terms of particular requirements.

Because of the relative simplicity of implementation and low computational cost, the MM has been extensively used by many researchers, and has become a powerful tool for investigating aerosol microphysical processes in most cases. The general disposition for this problem is to transform Eq. (2) into an ordinary differential equation with respect to the moment m_k. The moment transformation involves multiplying Eq. (2) by v^k and then integrating over the entire size distribution, and finally the transformed moment equations based on the size distribution are obtained:

$$\frac{dm_k}{dt} = \frac{1}{2}\int_0^{\infty}\int_0^{\infty}[(v + v_1)^k - v^k - v_1^k] \times \beta(v, v_1) n(v,t) n(v_1,t) dv\, dv_1 \quad (k = 0,1,2,\ldots), \tag{3}$$

where the moment m_k is defined by

$$m_k = \int_0^{\infty} v^k n(v) dv \tag{4}$$

In the past, some efforts have been made to achieve the closure of Eq. (3). Four prominent methods were proposed, i.e., making a priori assumption for the shape of the aerosol size distribution