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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:

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

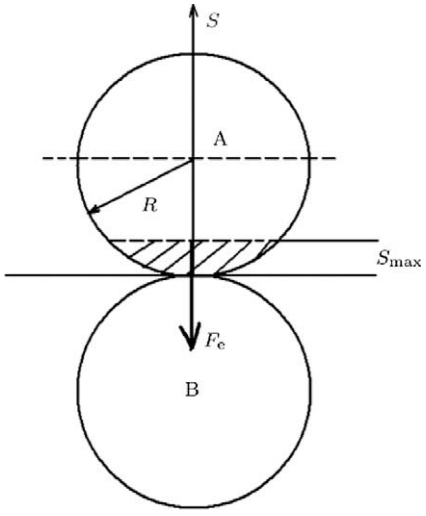

Fig. 1. Schematic diagram of the collision between two particles. R is the particle radius, while S_{max} is the maximum deformation.

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

(Pratsinis, 1988; Lee et al., 1984), approximating the integral moment by an n-point Gaussian quadrature (McGraw, 1997; Marchisio and Fox, 2005), assuming the pth-order polynomial form for the moments (Barrett and Jheeta, 1996), and achieving closure with interpolative method (Frenklach, 2002). Some of these methods have been evaluated and compared in accuracy and efficiency (Yu et al., 2008c). In our current studies, an alternative method, Taylor-expansion moment method (TEMOM), was proposed and has been proved to produce the accurate results with less computational cost (Yu et al., 2008c).

In order to apply the above methods to solving specific engineering problems, it needs to couple them with computational fluid dynamics, combustion kinetics and even chemical kinetics. In this section, we mainly address the newly proposed TEMOM method and in the next section show its potential in coupling with computational fluid dynamics.

3.1. Coagulation equation for spherical particulate system

The theory for solving Brownian coagulation process is transport theory based on Stokes' law and Einstein's diffusion theory in the continuum regime, and kinetic theory of gases in the free molecular size regime (Pratsinis, 1988). In the transient regime, however, one needs to introduce Fuchs's interpolation formula to approximate real values (Fuchs, 1964).

If the particle size falls into the free molecular size regime, then the collision frequency is obtained from the expression derived in the kinetic theory of gases (Friedlander, 2000):

$$\beta_{\mathrm{fm}}(v,v_1)=B_1(1/v+1/v_1)^{1/2}(v^{1/3}+v_1^{1/3})^2 \tag{5}$$

where $B_1=(3/4\pi)^{1/6}(6k_bT/\rho)^{1/2}$, k_b is the Boltzmann constant, T is the gas temperature and ρ is the mass density of the particles. It is necessary to rewrite Eq. (5) to be the following form, $\beta_{\mathrm{fm}}(v,v_1)=B_1(v+v_1)^{1/2}(v^{1/6}v_1^{-1/2}+2v^{-1/6}v_1^{-1/6}+v^{-1/2}v_1^{1/6})$. Here, it is convenient to expand $(v+v_1)^{1/2}$ about point ($v=u$, $v_1=u$) with first three terms. Then the collision frequency in free molecular size regime takes the following form,

$$\beta_{\mathrm{fm}}(v,v_1)=B_1\left(\frac{3\sqrt{2u}}{8}+\frac{3\sqrt{2}v}{8\sqrt{u}}+\frac{3\sqrt{2}v_1}{8\sqrt{u}}-\frac{\sqrt{2}v^2}{32u^{3/2}}-\frac{\sqrt{2}vv_1}{16u^{3/2}}-\frac{\sqrt{2}v_1^2}{32u^{3/2}}\right)\times\left(v^{1/6}v_1^{-1/2}+2v^{-1/6}v_1^{-1/6}+v^{-1/2}v_1^{1/6}\right) \tag{6}$$

As Eq. (6) is introduced into Eq. (3) and then closed by three-order Taylor-series expansion (Yu et al., 2008c),

$$m_k=\left(\frac{u^{k-2}k^2}{2}-\frac{u^{k-2}k}{2}\right)m_2+(-u^{k-1}k^2+2u^{k-1}k)m_1+\left(u^k+\frac{u^kk^2}{2}-\frac{3u^kk}{2}\right)m_0 \tag{7}$$

the system for first three moments can be finally written in the following form (Yu et al., 2008c):

$$\begin{cases}\dfrac{dm_0}{dt}=\dfrac{\sqrt{2}B_1(65m_2^2m_0^{23/6}-1210m_2m_1^2m_0^{17/6}-9223m_1^4m_0^{11/6})}{5184m_1^{23/6}}\\ \dfrac{dm_1}{dt}=0\\ \dfrac{dm_2}{dt}=-\dfrac{\sqrt{2}B_1(701m_2^2m_0^{11/6}-4210m_2m_1^2m_0^{5/6}-6859m_1^4m_0^{-1/6})}{2592m_1^{11/6}}\end{cases} \tag{8}$$

here, the expansion point of Taylor-series expansion takes the value, $u=m_1/m_0$ .If the particle size is approached to mean free path of the gas and falls into continuum plus near-continuum regime, the collision frequency is obtained from transport theory (Friedlander, 2000):

$$\beta_{\mathrm{co}}(v,v_1)=B_2\left(\frac{C(v)}{v^{1/3}}+\frac{C(v_1)}{v_1^{1/3}}\right)(v^{1/3}+v_1^{1/3}) \tag{9}$$

where $B_2=2k_bT/\mu$. The slip correction factor, $C(v)=1+A\cdot Kn$ ($A=1.591$), is used to accommodate the gas slip effects for small particles.

Similar to solution in free molecular size regime, the set of moment equations disposed by Taylor-series expansion technique can be obtained in this regime in the following:

$$\begin{cases}\left.\dfrac{dm_0}{dt}\right|_{\mathrm{co}}=B_2\left\{\dfrac{(-151m_1^4+2m_2^2m_0^2-13m_2m_1^2m_0)m_0^2}{81m_1^4}+\dfrac{\phi m_0^{7/3}(5m_2^2m_0^2-64m_2m_1^2m_0-103m_1^4)}{81m_1^{13/3}}\right\}\\ \left.\dfrac{dm_1}{dt}\right|_{\mathrm{co}}=0\\ \left.\dfrac{dm_2}{dt}\right|_{\mathrm{co}}=B_2\left\{-\dfrac{2}{81}\dfrac{-151m_1^4+2m_2^2m_0^2-13m_2m_1^2m_0}{m_1^2}-\dfrac{4}{81}\dfrac{\phi m_0^{1/3}(-2m_2m_1^2m_0-80m_1^4+m_2^2m_0^2)}{m_1^{7/3}}\right\}\end{cases} \tag{10}$$

where $\phi=A\lambda(4\pi/3)^{1/3}$. If the particle size is limited in continuum regime ($\phi=0$), Eq. (10) reduce to (Yu et al., 2008c):

$$\begin{cases}\left.\dfrac{dm_0}{dt}\right|_{\mathrm{co}}=B_2\dfrac{(-151m_1^4+2m_2^2m_0^2-13m_2m_1^2m_0)m_0^2}{81m_1^4}\\ \left.\dfrac{dm_1}{dt}\right|_{\mathrm{co}}=0\\ \left.\dfrac{dm_2}{dt}\right|_{\mathrm{co}}=B_2\left(-\dfrac{2}{81}\right)\dfrac{-151m_1^4+2m_2^2m_0^2-13m_2m_1^2m_0}{m_1^2}\end{cases} \tag{11}$$

It is obvious that Eqs. (8), (10) and (11) are all systems of first-order ordinary differential equations and all the right terms are denoted by the first three moments m_0, m_1 and m_2, and thus each system can be automatically closed. Under these conditions, the first three moments, which are also the three predominant parameters for describing aerosol dynamics, are obtained through solving this first-order ordinary differential system. Here, it should be pointed out that the whole derivation of the equations does not involve any assumptions for particle size spectrum, while the final mathematical form is much simpler than the PMM model.

3.2. Coagulation equation for fractal dimensional agglomerates

The above studies are limited to spherical particulate systems. For non-spherical particles such as aggregate and agglomerate, however, the description for their behaviors should be re-evaluated because the dynamics of non-spherical particles differs significantly from that of spherical particles. In fact, the dynamics of non-spherical particles is still a relatively new area (Friedlander, 2000).

Similar to spherical particles, there are also different collision kernels for aggregate or agglomerate in the free molecule regime and in the continuum regime, but the fractal dimension representing particle morphology should be additionally introduced. In the free molecule regime, the coagulation kernel is shown (Friedlander, 2000):

$$\beta_{\mathrm{nf}}(v,v_1)=E_1(1/v+1/v_1)^{1/2}(v^{1/D_f}+v_1^{1/D_f})^2 \tag{12}$$

where $E_1=(6k_bT/\rho)^{1/2}(3/4\pi)^{\lambda}a_{p0}^{2-6/D_f}$, D_f is fractal dimension, and a_{p0} is the radius of primary particle. Substituting Eq. (12) into Eq. (3) as well as performing 3-order Taylor-series expansion for fractal moment terms, we got the following 3-order set of moment equations for agglomerates:

$$\begin{cases}\dfrac{dm_0}{dt}=-\dfrac{E_1}{2}[\xi_1^*\phi_1+\xi_2^*\phi_2+\xi_3^*\phi_3]\\ \dfrac{dm_1}{dt}=0\\ \dfrac{dm_2}{dt}=\dfrac{E_1}{2}[\varsigma_1^*\phi_1+\varsigma_2^*\phi_2+\varsigma_3^*\phi_3]\end{cases} \tag{13}$$

here ξ_1^*, ξ_2^*, ξ_3^*, ς_1^*, ς_2^* and ς_3^* are comprised of fractal moment variables shown in reference (Yu and Lin, 2009b), $\phi_1=3\sqrt{2u}/8$,

$\phi_2 = 3\sqrt{2}/8\sqrt{u}$, $\phi_3 = -\sqrt{2}/32u^{3/2}$ and u is the expansion point of Taylor-series expansion. It is well known that Eq. (13) cannot be automatically closed because this set of equations is essentially comprised of fractional-order moments, not integral moments. In order to break this limit, it is necessary to follow our previous disposition for spherical collision (Yu et al., 2008c) and use Eq. (6) to achieve the closure. If the fractional dimension in Eq. (13) takes the value 3, it ultimately reduces to Eq. (8) for classic spherical collision. The expansion point takes the following expression, $u = m_1/m_0$.

Similarly, by performing Taylor-series expansion for unintergral and fractional terms in transformed moment equations, we can also obtain the moment equations for agglomerate coagulation in the continuum regime. In this regime, the collision kernel is (Friedlander, 2000):

$$\beta_{\mathrm{nc}}(v, v_1) = B_2\left(\frac{1}{v^{1/D_f}} + \frac{1}{v_1^{1/D_f}}\right)\left(v^{1/D_f} + v_1^{1/D_f}\right) \tag{14}$$

and the Taylor-series expansion moment equations for non-spherical collision in the continuum regime:

$$\begin{cases} \frac{dm_0}{dt} = B_2\frac{-m_0^2(-5f^2m_1^4+f^4m_1^4+8m_1^4+f^4m_2^2m_0^2-2f^4m_2m_1^2m_0+6f^2m_2m_1^2m_0-f^2m_2^2m_0^2)}{4m_1^4} \\ \frac{dm_1}{dt} = 0 \\ \frac{dm_2}{dt} = B_2\frac{-5f^2m_1^4+f^4m_1^4+8m_1^4+f^4m_2^2m_0^2-2f^4m_2m_1^2m_0+6f^2m_2m_1^2m_0-f^2m_2^2m_0^2}{2m_1^2} \end{cases} \tag{15}$$

where $f = 1/D_f$. Here, Eq. (15) ultimately reduce to Eq. (11) if f takes the value 1/3, i.e., $D_f = 3$.

In order to apply the TEMOM to entire size regime, it is necessary to combine moment equations in the free molecule regime with equations in the continuum regime by harmonic mean solution or Dahneke's solution (Otto et al., 1999). Following this solution, Yu and Lin (2009a) studied agglomerate coagulation due to Brownian coagulation in the entire size regime. They found the TEMOM model disposed by Dahneke's solution (TEMOM-Dahneke) is more accurate than by harmonic mean solution (TEMOM-Harmonic) through comparing their results with the reference sectional model (SM) for different fractal dimensions. In the transition regime, the TEMOM-Dahneke gives more accurate results than the quadrature method of moments with three nodes (QMOM3). The mass fractal dimension was found to play an important role in determining the decay of agglomerate number and the spectrum of agglomerate size distribution. They also found the self-preserving size distribution (SPSD) theory and linear decay law for agglomerate number are only applicable to be in the free molecular regime and continuum plus near-continuum regime, but not perfectly in the transition regime.

4. Evolution of nanoparticle dynamic in coherent structures

Many existing studies on particulate dispersion in turbulent jet flows are usually based on time-averaged flow models. However, coherent structures, which are wiped out by average, exist in jet flows. These coherent structures play a significant role in the momentum and energy transport in the flows. In the multiphase flows, contrary to the dispersion of particles in isotropic homogeneous turbulence, the particle dispersion in jet flows is strongly dependent of the forming, growth and interaction of coherent structures in the flow. Therefore, some research literatures have been devoted to the dispersion of particles in the turbulent jet with coherent structures. But those studies were related just to the dispersion of coarse solid particles in jet flows, in which the phenomenon such as particle coagulation was not considered. The work on the dispersion of nanoparticle in the jet with coherent structures is little reported yet in author's knowledge. Here, we review our recent studies on interaction between the coherent structures and the nanoparticle coagulation and dispersion process in nanoparticle-laden multiphase jet flows.

4.1. Nanoparticle coagulation in a planar jet flow

Studies on the connection between nanoparticle dynamics a coherent structures have been generally limited. To authors' knowledge, the relevant works were first performed by the group of Garrick (Garrick et al., 2006; Settumba and Garrick, 2003; Wang and Garrick, 2005) by coupling direct numerical simulation (DNS) (or large eddy simulation (LES)) and moment method (or sectional method) for mixing layer and jet flow. Similarly, the spatial temporal evolution of nanoparticle dynamics in a planar free jet flow was studied by Yu et al. (2006) as shown in Fig. 2. In their studies, the LES was utilized to obtain the flow information while the log-normal moment method (Lee et al., 1984) to obtain the evolution of nanoparticle dynamics in coherent structures. This type of flow occurs more commonly in industry and natural environments than temporal mixing layers. The numerical simulation showed that coherent structure dominates the distributions of particle number intensity, mass concentration, size distribution and polydispersity, and increases the diffusion of particles into the surroundings. As the Damköhler number (D_a) was introduced, Yu et al. (2007b) found the larger the Damkohler number, the higher the polydispersity, which is shown in Fig. 3.

4.2. Nanoparticle coagulation and diffusion in a planar impinging jet flow

Unlike the free jet flow, impinging jet flow will lead to more complicated flow structures due to the presence of impinging plane. The schematic of nanoparticle-laden impinging jet is shown in Fig. 4. Earlier studies in this field were limited in experimental research for capturing the evolution of coherent structures and examining the particle deposition without considering the instantaneous influence of coherent structures on the nanoparticle dynamics.

In order to deeply understand the evolution of nanoparticle dynamics with time in coherent structures, Yu et al. (2007a) studied the effect of Reynolds number and nozzle-to-plate distance on the distribution of particle dynamics such as number and mass concentration, and polydispersity. In their works, the combination of the LES and the QMOM (McGraw, 1997) was performed. It was found that increasing of Reynolds number results in an increase in particle number concentration and a decrease in particle size, and similar results arise from decreasing nozzle-to-plate distance. One of the results is shown in Fig. 5.

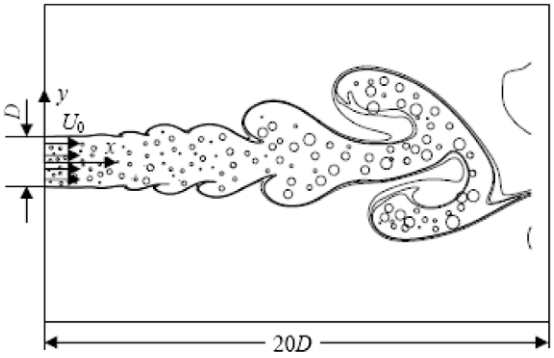

Fig. 2. Schematics of nanoparticle-laden planar jet.

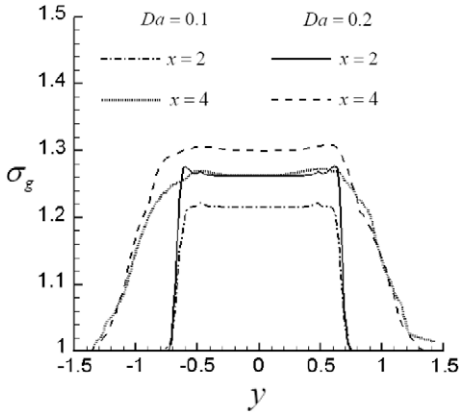

Fig. 3. σ_g for different Da at different axial positions.

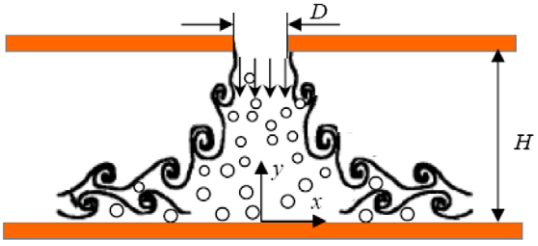

Fig. 4. Schematic diagrams of a planar impinging flow.

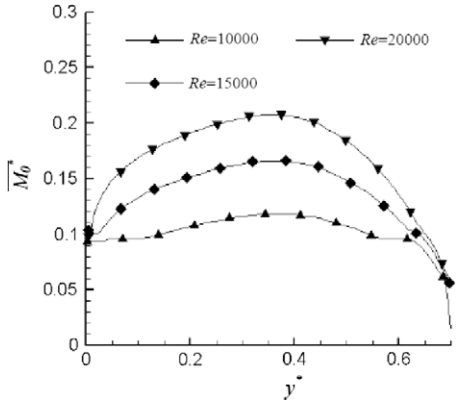

Fig. 5. Effect of Reynolds number on particle number intensity.

4.3. Nano and fine particle coagulation and dispersion in a round jet

Available studies have shown the mechanism and characterization of particle dispersion in turbulent flows are quite different for nano and fine particles. For the fine particles, Stokes law is capable of predicting the dynamic microstructural properties as well as macroscopic properties in either dilute or concentrated, while for the nanoparticles, the general dynamic equation may be preferential. In the existing investigations, fine particles and nanoparticles are usually treated separately, and there is few available models for predicting the interaction between them.

In the Chan and his colleagues' study on round multiphase flow (Chan et al., 2006), the fine particles were traced with the Lagrangian method while the nanoparticles were described with the Eulerian method. The discrete vortex method together with a technique of vortex filament augmentation and amalagamation was used to simulate a round jet flow shown in Fig. 6. In order to close particle

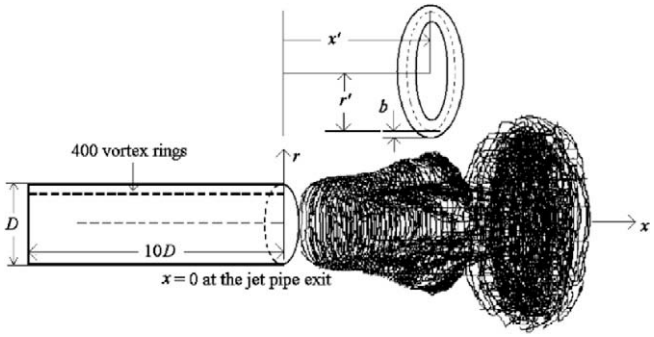

Fig. 6. Schematic diagrams of flow simulation geometry and vortex ring.

general dynamic equation, the log-normal moment method (Lee et al., 1984) was used. This solution was capable to simultaneously calculate the trajectories of individual fine particles and the distribution of nanoparticle dynamics, and thus overcome the limitation of the earlier researchers' works. In order to take into consideration the effect of the fine particles on the gas flow, a model based on the modified velocity was developed,

$$\Delta u = \frac{R_s - r_g}{R_s}\Delta u_c = -\frac{4}{27000}\frac{\rho_p}{\rho_g}\frac{R_s - r_g}{R_s}\Delta u_p \tag{16}$$

where Δu is the velocity variation of fluid at r_g within the volume, Δu_c is the velocity variation of fluid at the central point of volume, R_s is the radius of a spherical fluid volume, r_g is the distance from the central point to the border within the volume, ρ_g is the gas density and ρ_p is particle density. A perturbation terms was added to the flow to accelerate the development of the large-scale vortex structures,

$$d_s = r'[1.0 + a_m \sin(\alpha\phi)] \tag{17}$$

here, d_s is the distance from the initial vortex segment to the centerline of the jet, r' is the radius of vortex ring, a_m is the amplitude of the perturbation, α is the azimuthal perturbation wave number and ϕ is the azimuthal angle.

Chan et al. (2006) explored the effect of particle Stokes number, perturbation wavenumber, and amplitude on the dispersion of fine particles, and the dispersion and dynamics of nanoparticles in a round jet. One of the important results is shown in Fig. 7. Using a similarity solution, Lin et al. (2007) explored the effect of coherent structures on nanoparticle dispersion and coagulation in a round jet, and found the coherent structures play an important role in enhancing the particle collision and transport along the direction, and making the particles dispersion non-uniformly along the stream direction.

5. Specific engineering problems

The numerical technique by coupling computational fluid dynamic with population balance modeling has become an important tool to investigate nanoparticle synthesis, combustion, environment pollution, fluidized beds, biology process, etc. In theory, these problems involve multi-dimensional multi-species turbulent flows with strong mass and energy coupling between the phases. Therefore, understanding such processes requires detailed knowledge of complex fluid behavior coupled with transport and dynamics of carrying phase and dispersed phase. In this filed, special attention was usually paid to developing more appropriate numerical model for particle dynamics as well as flow field.

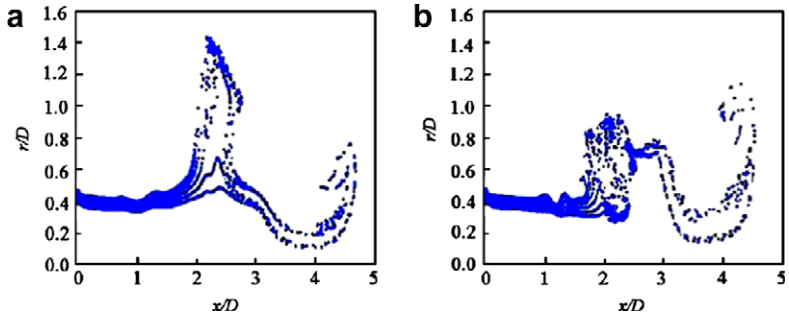

Fig. 7. Fine particle dispersion at $\tau = 15$ and $St = 0.05$ for different wavenumbers: (a) $\alpha = 5$; (b) $\alpha = 9$.

5.1. Non-spehrical nanoparticle synthesis in a combustion flow

The synthesis of TiO_2 nanoparticles mostly occurs in a diffusion flame reactor by gas-to-particle conversion. The fundamental physics of non-spherical particle evolution in a flame reactor is still limited because the complex interplay between diffusive mixing (i.e., fluid-dynamic, thermal and chemical processes) and particle growth in synthesis is difficult to be observed experimentally. To predict the characteristics of synthesized nanoparticles, it needs to develop an efficient mathematical model by combining the flame dynamics with particle kinetics theory to accurately simulate the formation and growth of particles. The shape of particles is not spherical and thus the morphology should be exhibited in the population balance equations.

To accomplish this aim, Yu et al. (2008a) proposed a computational model combining the fluid dynamics with the particle kinetics in which the momentum, heat, and mass transfer, Brownian coagulation and diffusion, surface growth, coalescence and thermophoresis were simultaneously taken into account. An efficient quadrature method of moments (McGraw, 1997) was allowed to approximate the general dynamics equation, and the eddy dissipation concept (EDC) combustion model (Magnussen, 1981) was used to estimate the flame temperature field. The particle size and surface were treated as independent variables. The configuration of the burner numerically is shown in Fig. 8 in which TiO_2 initially arisen from the decomposition of Titanium tetraisopropoxide (TTIP). The results showed the maximum particle number occurs in front of the high temperature zone because of high precursor reaction rate, and then decreases due to coagulation, as shown in Fig. 9. Similar trends were also found in the total surface area, the geometric standard deviation and the primary particle number per agglomerate. This work also revealed that coalescence has more effect on final produced particle morphology than coagulation. An analysis of the geometric standard deviation showed the distribution of the final produced particles for flame reactor can reach self-preserving state, which is consistent with the experimental results.

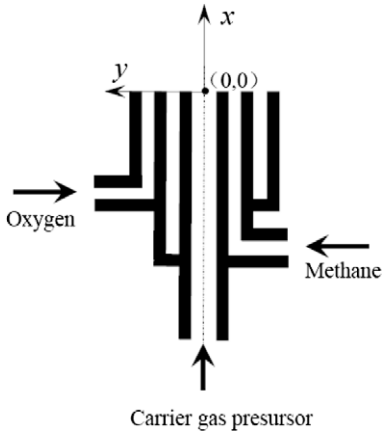

Fig. 8. The configuration of the burner.

Following a similarity solution, Yu et al. (2008b) also numerically investigated the synthesis process of TiO_2 as $TiCl_4$ vapours were taken as precursor, and studied the effect of precursor loading on TiO_2 agglomerate dynamics in a diffusion flame reactor. Similarly, the independent method for treating particle size and surface was applied. In order to associate particle surface area with particle size, Yu et al. (2008b) proposed to use the following relationship:

$$A_{\min} = (\pi m_0)^{1/3} (6 m_1)^{2/3} \tag{18}$$

where A is the particle surface area concentration, m_0 and m_1 are the number and mass concentration, respectively.

They found that increasing precursor loading leads to the larger agglomerated particles with a broader size distribution. The effect of precursor loading on primary particles was also revealed in that the primary particle number and size increase with the increasing of precursor loading, while the total specific surface area decreases. More importantly, their numerical simulation further proved that particles with more irregular shapes have more chances to coagulate and form larger agglomerates.

5.2. Particulate formation in diesel exhaust plumes

In atmospheric environment and industry exhausts, it has been realized that some nanoparticles come from multi-component route, i.e., binary homogeneous nucleation process of water–sulfuric acid vapours, whereas a complete theoretical understanding of this phenomenon is still a challenge due to its complicated chemical/physical processes. With increased computing power, it is increasingly possible to simultaneously capture details of the fluid flow and transport, and the evolution of the water–sulfuric acid nanoparticle dynamics.

This problem has been sufficiently investigated by many researchers using numerical methods, but the coupling between computational fluid dynamic and particle dynamic is not yet enough. In order to grasp the nature of particle formation and growth in a turbulent diesel exhaust plume, the coupling between TEMOM and LES was performed by Yu et al. (2009c). The numerical moment equation based on Taylor-series expansion was:

$$\frac{dm_k}{dt} + \frac{d(\overline{u}_j + (u_{th})_j) m_k}{dx_j} = \frac{d}{dx_j}\left((\Gamma_t + \Gamma_B) \frac{dm_k}{dx_j} \right) + k B_1 \hbar m_{k-1/3} \times \frac{x v_a + (1-x) v_w}{x v_a} + J(v^*) v^{*k} + \left[\frac{dm_k}{dt} \right]_{coa} \quad (k = 0, 1, 2) \tag{19}$$

where u is gas velocity, Γ_B and Γ_t are Brownian and turbulent diffusion coefficient, v_a and v_w are the sizes of sulfuric acid molecule

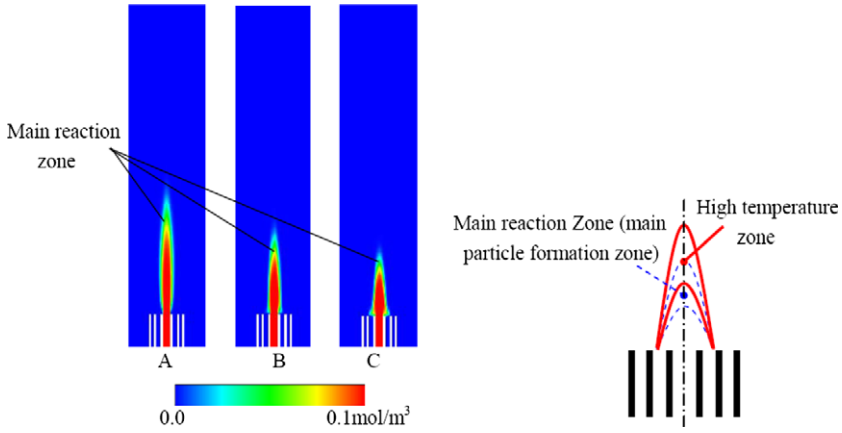

Fig. 9. Mole concentration of the TTIP at different oxygen flow rate.

and water molecule, x is the volume fraction of sulfuric acid in particles. The nucleation rate $J(v^*)$ was from Vehkamaki's parametrized model (Vehkamaki et al., 2003), and the kth moment derivative, $[dm_k/dt]_{coa}$, was obtained from Eq. (8). Compared to other published numerical methods, the present TEMOM requires the least computational time with much accuracy for predicting nanoparticle dynamics. It was found besides the flow convection and diffusion, fuel sulfur content, relative humidity and temperature are three other key parameters influencing nanoparticle formation and growth. By investigating geometric standard deviation, nucleated particles were shown to eventually approach the self-preserving distribution in the dilution atmosphere. Similarly, Yin et al. (2008) also combined the LES with the general dynamic equation to study the nucleation and coagulation process of nanoparticles in parallel twin jets. They found gas-to-particle conversion mostly takes place in the middle and interface of the twin jets, and the higher the sulfur content, the greater the number of nanoparticles.

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