NUMERICAL MODELING OF FINE PARTICLE FRACTAL AGGREGATES IN TURBULENT FLOW

by

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A method for prediction of fine particle transport in a turbulent flow is proposed, the interaction between particles and fluid is studied numerically, and fractal agglomerate of fine particles is analyzed using Taylor-expansion moment method. The paper provides a better understanding of fine particle dynamics in the evolved flows.

Key words: *fractal aggregates, fine particles, turbulent flows, porosity, permeability*

Physical models of kinetic coagulation

Fine-particle-laden multiphase flow is an important research area in the field of multiphase flows. A thorough understanding of the nature of fine particle transport and the strong coupling with carrier fluid phase is of great practical importance. Examples include accurate predication of air pollution index, and effective control of desirable particulate transport [1]. In physics, the study on fine particle-laden multiphase flow belongs to the field of mesoscopic theory. This type of problems has unique characteristics including its temporal unsteady-state and spatial non-equilibrium. The evolution and dynamics of particulate flows are significantly influenced by some non-linear, unsteady, multi-scale chemical, and physical processes as well as strong coupling between phases [2]. Nowadays, the existing theories of fine-particle-laden multiphase flow have some shortcomings, such as the disharmony of computational efficiency and accuracy.

In theory, the evolution of aerosol size distribution in the flow field can be highly traced by solving the particle general dynamic equation (PGDE). The PGDE equation has an ability to describe the combined physical processes for ultrafine particles. Unfortunately, the general dynamic equation has a limited number of known analytical solutions only, due to its non-linear integro-differential structure [3]. Hence, an alternative method, *i. e.* the numerical technique, has to be applied to obtaining approximate solutions to this equation [4]. However, the numerical simulations often become impractical even with a modern super-computer, due to the large computational cost [5].

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Based on homogeneous, isotropic turbulence with spherical particles smaller than the Kolmogorov microscale [6] (for which particle inertia can be neglected), the turbulent gradient of mean square root velocity is:

$$\overline{\left(\frac{\partial u_i}{\partial x_j}\right)^2} = \frac{2\varepsilon_t}{15\nu} \tag{1}$$

The collision kernel for two particles or aggregates can be caused by the ever-present Brownian motion or by shear deformation of the fluid. Here, only particles of at least micron sizes are considered. In this case, the effect of Brownian motion is negligible compared to shear.

Generally, aggregates are considered as spherical particles, the shearing movement causes the orthokinetic coagulation [7], and its collision frequency function is:

$$\beta_{\mathrm{SH}}(\nu, \varepsilon) = \frac{k_s}{\pi}\sqrt{\frac{\varepsilon_t}{\nu}}\left(\nu^{\frac{1}{3}} + \varepsilon^{\frac{1}{3}}\right)^3 \tag{2}$$

However, in fact, aggregates are irregularly shaped with a void fraction or inversely an aggregate density that depends on aggregate size. As the aggregates exhibit fractal-like properties, they can be characterized by a fractal dimension D_F. In sheared suspensions the fractal dimension is typically in the range of 2.1~2.7 [8, 9]. Here, the fractal dimension is a constant. Consequently, the fractal dimension and primary particle size can be considered as averaged values for all particles of the aerosol, irrespective of agglomerate size. The collision frequency function is expressed as:

$$\beta_{\mathrm{SH}}(\nu, \varepsilon) = \frac{k_s}{\pi}\sqrt{\frac{\varepsilon_t}{\nu}}\,\nu_0^{1-\frac{3}{D_\mathrm{F}}}\left(\nu^{\frac{1}{D_\mathrm{F}}} + \varepsilon^{\frac{1}{D_\mathrm{F}}}\right)^3 \tag{3}$$

The moment transformation includes multiplying Smoluchowski's discrete coagulation equation governing the continuous size distribution of the number concentration function, which is developed by Muller in 1928, by v^k, and integrating over the entire size distribution. Finally, the transformed moment equations based on the size distribution are obtained [5, 10].

Under these conditions, the first three moments, which are also the three predominate parameters describing fine-particulate dynamics, are obtained by solving the first-order differential equation system. It is worth noting that the whole derivation of the equations does not involve any assumptions on particle size spectrum, while the final mathematical form is much simpler than that from the particle moment method (PMM) model.

Results and analysis

The effectiveness of the shear-induced flocculation is strongly dependent on surface and colloid chemistry of the system. The Kolmogorov microscale $\eta = (\upsilon^3/\varepsilon_t)^{1/4}$, characterizing the length scale of the energy dissipating turbulent eddies. For fine particulate matter as small as about 100 microns, the random nature of a turbulent flow affects a particle only in a fairly simple way. The particles are smaller than the smallest eddies of the turbulence, which are measured by the Kolmogorov length. The turbulent flow field is heterogeneous and well characterized by a turbulent shear only when particles are smaller than η. Cleasby [11] suggested that the coagulation of particles larger than η correlated best with $(\varepsilon_t)^{2/3}$ versus $(\varepsilon_t)^{1/2}$ from calculations of the root mean square eddy velocity difference and observed good agreement with literature data. Clark [12] suggested that while a mean velocity gradient characterizing the average coagulation rate may exist. Glasgow *et al.* [13] showed that the local turbulent energy dissipation rate can exceed the average value by an order of magnitude depending on the surrounding velocity. It is suggested that based on the Kolmogorov theory of local isotropy, local turbulent energy dissipation rates are proportional to the average value, ε_t.

However, this assumption is valid in the viscous sub-range of the turbulence. In a full turbulent flow, the collision of particles results not only from the shear gradient of fluid velocity in the viscous sub-range, but also from the subsequent movement of particles to different vortices incoherent from each other in the inertial sub-range, especially when the particle size is larger than the Kolmogorov microscale η. Taking this into account, the aggregation rate equation has been modified such that the turbulent shear rate is characterized by the average velocity gradient or shear rate, the same as in laminar flow.

The average shear rate is given in terms of the turbulent dissipation rate ε_t and kinematic viscosity υ. This coefficient takes different forms depending on particle size relative to the smallest eddies in the fluid. Smallest eddy size in the fluid is termed as the Kolmogorov scale. Oceanic dissipation rates span many orders of magnitude from 10^{-6} to 10^2 cm$^2 s^{-3}$. Therefore the minimal eddy size indicated by this calculation may be as large as 1 cm or as small as 10^{-2} cm. Most marine particle sizes range from sub-micrometer scales, indicating the importance of kernel expressions for particles smaller than the Kolmogorov scale [14].

Equations (1)-(3) assume that the turbulence intensity is sufficiently large that the flow field may be considered homogeneous. As a result, the suspended particles are flung randomly from eddy to eddy and collide.

As it is already known, aggregates are now recognized to exhibit fractal properties and, as such, may be expected to form somewhat different behavior from non-aggregated particles. Generally, the fractal dimension is the measure of how to fill floc space by particles. The fractal nature of aggregates has two effects that are important for coagulation modeling: it makes them bigger for a given mass, and it alters the fluid flow through them. Because the particles are bigger, the coagulation kernels describing their interactions change. One implication of these influences of fractal particulate aggregates is that the porosity of the aggregate is not spatially uniform. Such behavior is certain to influence the permeability of the aggregate and suggests that factors such as fractal dimension coupled with aggregate size are important to the aggregates properties. The porosity and the permeability can be determined using Happel models [15]. For the aggregates with fractal dimension D_F = 1.9 and 2.3, they are shown in figs.1(a) and (b) as functions of the dimensionless aggregate volumes. Shear contact occurs when different parts of the fluid move at different speeds relative to each other, and thus a particle moving with a faster fluid patch overtakes and collides with a particle in a slower fluid patch. The porosity increases as the volume of the aggregates increases and as the fractal dimension decreases, fig. 1(a). An aggregate with fractal dimension less than three has weaker space filling ability, which results in larger porosity. When the porosity is higher than zero, water is incorporated inside the aggregate structure. An aggregate is assumed to be characterized by a uniform effective internal permeability corresponding to its average porosity.

Discussions and conclusions

Recently, Maricq [16] applied the sectional method to investigate the evolution of fractal-like particles in the transition regime by performing Harmonic mean solution, and found both the shapes and temporal evolution of the soot size distributions can be well reproduced.

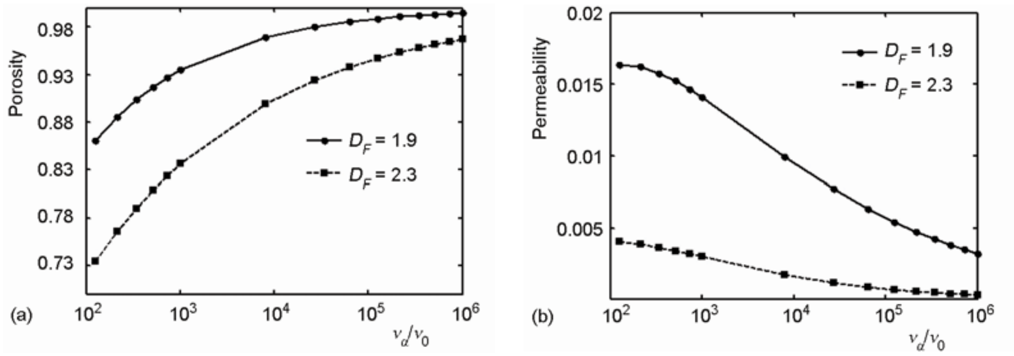

Figure 1. Effects of fractal dimension on porosity and permeability as functions of aggregate volume; (a) porosity, (b) permeability

In order to break the limitation in computational cost, the moment method (MM) is usually used, and it has become a powerful tool for predicting microphysical processes of fine particle aggregates in many cases. But it is still difficult to be extended to agglomerates due to the presence of fractal dimension. In the studies on the relationship between the fractal dimension and the dynamics of agglomerates, our previous studies [5, 10, 17], an alternative method named Taylor-expansion moment method (TEMOM) was proposed and proved accurate with less computational cost. This method has both advantages and disadvantages in accuracy and efficiency, and now they are used in different fields in terms of the particular requirement. Although the sectional method is computationally tractable with high accuracy, there is still a need to use the TEMOM method to solve aerosol coagulation process since it is more efficient than the former. More importantly, it does not lose much accuracy without the prior requirement of the particle size distribution spectrum. Here, we extend this method to agglomerate coagulation due to turbulent shear mechanism.

The results show that the partial 4^{th}-order Taylor expansion method of moments can be applied to analyze the problem involving fine particle turbulent shear coagulation with high accuracy, and the self-preserving size distribution is found in fine particle-laden multiphase systems dominated by turbulent shear.

In conclusion, this paper is mainly focused on the development of improved MM and the extension of the scope of the classic Smoluchowski mean-field theory. The method can be used to provide a better understanding of the nature of fine particle dynamics in the evolved flows.

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Nomenclature

D_F – fractal dimension
k_s – shear constant
u – velocity [cm s^{-1}]
v_0 – volume of primary particle [cm^3]
v, ε – particle volume [cm^3]

Greek symbols

β_{SH} – collision frequency function [cm^{3}s^{-1}]
ε_t – turbulent dissipation rate [cm^{2}s^{-3}]

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