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The self-preserving size distribution of fractal aggregates coagulating by Brownian motion and simultaneous fluid shear at low Peclet numbers: Numerical solutions

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ABSTRACT

The asymptotic size distribution of fractal particles undergoing Brownian and simultaneous shear-induced coagulation has not been investigated. We have addressed this issue by establishing and solving ordinary integro-differential coagulation equations. The self-preserving distribution (SPSD) requires a shear rate decreasing with time according to a formula, which we report, for various fractal dimensions. Under this condition, it is the Peclet number of primary particles that controls the self-preservative characteristics of coagulating aggregates. The size distribution of fractal aggregates at low Peclet numbers of primary particles was determined to be self-preserving. The SPSDs were calculated for aggregates of various fractal dimensions. An upper limit of the Peclet number exists where the SPSD could be obtained. This upper limit decreases with decreasing fractal dimension: from 1.1 for the fractal dimension of 3 to 0.14 for the fractal dimension of 1.8. The Peclet number of particles with the mean volume hydrodynamic radius is a constant during the coagulation process, and is proportional to the Peclet number of primary particles. As the Peclet number increases, the SPSDs will broaden, and the peak value will also increases and drifts to the left. The SPSD is close to a lognormal distribution. This represents a theoretical foundation for the size distribution evolution of coagulating fractal aggregates in flow fields and for the lognormal size distribution assumption of atmospheric aerosols.

1. Introduction

Coagulation kinetics and the evolution of the resulting particle size distribution are of importance in aerosol science, medicine, and industrial processes such as particle production in industrial aerosol reactors. As the particles grow and become larger, the particle size distribution evolves gradually. Coagulation processes are controlled by Smoluchowski's coagulation equation. The self-preserving solution to Smoluchowski's coagulation equation exists under some conditions. This self-preserving solution is an asymptotic solution toward which all systems converge, regardless of the initial distribution. The coagulation that leads to a self-preserving size distribution (SPSD) is called a self-preserving coagulation in this paper. The self-preservation of the size distribution of coagulating particles is determined by the homogeneity of the collision frequency function $\beta(u,v)$ (Menon & Pego, 2004). In general, for a large class of homogeneous kernels $\beta(\lambda u,\lambda v)=\lambda^{\gamma}\beta(u,v)$ with $\gamma<1$, there is numerical evidence

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that solutions evolve to a self-preserving form (Lee, 2001). There are also physical self-consistency arguments that have been used to derive the asymptotics for scaling solution (van Dongen & Ernst, 1988).

For Brownian coagulation ($\gamma=0$), a similarity transformation of the size distribution of spherical particles has been shown to lead to a SPSD in the continuum regime after a sufficient time (Friedlander & Wang, 1966). Similarly, studies have shown that SPSDs also exist for fractal particles undergoing Brownian coagulation. The SPSDs for fractal particles in the continuum and free molecular regimes were calculated by solving the complete population balance equation using a sectional method (Vemury & Pratsinis, 1995). Dekkers and Friedlander (2002) derived the ordinary integro-differential equations of Brownian coagulation for fractal particles and applied these equations to calculate the SPSDs in the continuum and free molecular regimes, and quasi-self-preserving size distributions in the near-continuum transition regime.

For shear-induced coagulation, the collisions induced by Brownian motion and the collisions induced by fluid shear should be considered simultaneously although pure shear-induced coagulation does not lead to a SPSD (Pratsinis, 1989). Wang and Friedlander (1967) have determined that the coagulation of spherical particles induced by the combination of Brownian motion and fluid shear can lead to a SPSD provided that the shear rate decreases with time according to a formula.

The self-preservation of particle size distributions provides an efficient method for solving Smoluchowski's coagulation equation. It brings a simplification of mathematical description and facilitates process design through computational fluid and particle dynamics (Johannessen, Pratsinis, & Livbjerg, 2001). Furthermore, lognormal distribution is usually used to describe atmospheric aerosol population size distribution (Hinds, 1999; Lee, Chen, & Gieseke, 1984; Park, Lee, Otto, & Fissan, 1999; Pratsinis, 1988). It is interesting that whereas the average size and the width of an aerosol size distribution strongly depend upon the chemical composition, the generation and the age of each aerosol, the basic shape of an aerosol size distribution is usually very close to a log-normal distribution or to a linear combination of different lognormal distributions (Seinfeld & Pandis, 2006). However, there is hardly any theoretically and statistically detailed explanation for this practice although there are some investigations on this problem for aerosol particles undergoing Brownian coagulation (Friedlander & Wang, 1966; Otto, Fissan, Parkt, & Lee 1999) and for the nucleation and growth processes (Bergmann & Bill, 2008; Kiss, Söderlund, Niklasson, & Granqvist, 1999).

As noted, studies show that the size distribution of spherical or fractal particles undergoing Brownian coagulation are self-preserving unconditionally. The self-preservation of size distribution of spherical particles undergoing Brownian and simultaneous shear-induced coagulation requires a special decreasing shear rate. Nevertheless, coagulation processes are often accompanied by fluid flow and the particles have a fractal structure (Xiong & Friedlander, 2001). To the best of our knowledge, the asymptotic size distribution of fractal particles undergoing Brownian and simultaneous shear-induced coagulation has not been investigated. We have addressed this issue by deriving and solving the ordinary integro-differential coagulation equations for the SPSD of fractal particles undergoing coagulation induced by the combination effect of Brownian motion and fluid shear at low Peclet numbers. The results may provide a theoretical foundation for the size distribution evolution of coagulating fractal particles in flow fields and the lognormal size distribution assumption of atmospheric aerosols.

2. Theory

2.1. Coagulation equations

The Polish physicist Smoluchowski (1917) published the first model of the coagulation process, which is given by

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

where $n(v,t)$ is the number concentration of particles with volume v to $v+dv$ at time t; and $\beta(v,\tilde{v})$ is the collision frequency or collision kernel between particles with volume v and $\tilde{v}$. The form of $\beta(v,\tilde{v})$ depends on the mechanisms of collision, which include Brownian motion, fluid shear, and differential sedimentation.

The process of coagulation usually is associated with sintering of the resulting aggregates. The term sintering refers to the coalescence of connected particles through neck formation. Sintering is not significant at low temperatures. Therefore, sintering of aggregates is not considered in Eq. (1) due to a restricted focus on the coagulation process in low temperature media. In addition, Eq. (1) also excludes the breakup of aggregates although it has been known to occur for particles larger than the Kolmogorov scale.

If the collision frequency is a homogeneous function of particle volume, Eq. (1) can be converted into an ordinary integro-differential equation with η as an independent variable by introducing the self-preserving dimensionless variables (Friedlander, 2000)

$$\eta=\frac{v}{\overline{v}},\quad n(v,t)=\frac{N(t)}{\overline{v}}\psi(\eta)\text{ with }\overline{v}=\frac{\phi}{N(t)} \tag{2}$$

where η is the dimensionless particle volume; $\psi(\eta)$ is the dimensionless number distribution function; $\overline{v}$ is the number average particle volume, and ϕ represents the volumetric particle fraction; $N(t)$ is the total number of particles per unit