Contents lists available at ScienceDirect

Chemical Engineering Research and Design

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

Perikinetic and orthokinetic aggregation of small solid particles in the presence of strong repulsive forces

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ARTICLE INFO

Article history:
Received 31 January 2018
Received in revised form 11 May 2018
Accepted 13 June 2018
Available online 21 June 2018

Keywords:
Aggregation kernel
DLVO
Extended DLVO
Hydrophobic effects
Particle–bubble interactions

ABSTRACT

This paper deals with aggregation of small particles in a fully developed turbulent flow field for the wide range of the Péclet number including the perikinetic and orthokinetic regimes. Colloidal particles smaller than the Kolmogorov length microscale are considered. Convective movements of these particles are characterised by the relaxation time much shorter than the Kolmogorov time microscale. A basic aggregation kernel is determined by solving the convection–diffusion equation for the pair probability function of the solid particles present in the DLVO potential field for the sub-Kolmogorov scale flow structure. The simplified aggregation kernels are proposed as well to offer a computationally less expensive method. An aggregation kernel based on the modified Fuchs stability ratio approach including effect of competition between maximum particle velocities caused by the repulsion forces and fluid flow is derived using a concept of small scale turbulent diffusion that competes with particle velocity generated by repulsion forces. The aggregation rate constants obtained using this method are close to predictions of the full model. Proposed approach is extended to take into account hydrophobic effects and particle-bubble interactions.

1. Introduction

There is a growing interest in the development of applications using fine and ultrafine particles as final or intermediate products in different industries dealing with chemicals, pharmaceuticals, cosmetics, food processing materials, etc. The main advantage of the use of these particles lies in their increased reactivity due to the increase in their surface-to-volume ratio. Fine particles of this property can be used to design highly efficient surface active materials by coating surfaces with a layer of particles having desired properties, for example antibacterial. However, the manufacturing process should be designed in a way that prevents the reemission of the nanoparticles to the environment during life cycle of the product (Bressot et al., 2017a, 2017b). These specific properties give rise to many studies on the fundamental level because fine particles offer broad industrial perspectives. The performance of particulate products such as fluidity, formability, optical properties, reactivity, etc. will depend on the size and surface properties of the particles. For this, exact knowledge of their structural features is essential when developing fabrication technologies and searching for new types of nanostructures or nanoparticles with specific properties. For the latter, the knowledge of the precise temporal evolution of the growth and aggregation processes is fundamental when it comes to industrial production and applications. The modelling of such phenomena still remains a real scientific and industrial challenge due to complex mechanisms and large number of process parameters influencing the system evolution, i.e. temperature, pH, salt concentration, type of ions present in the system and parameters determining flow, mixing and mass transfer. Effects of salt concentration and type of ions, including their valence, on interaction forces and aggregation rates of latex particles and titanate nanowires have been examinedexperimentally

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https://doi.org/10.1016/j.cherd.2018.06.021

by several workers using dynamic light scattering and colloidal probe technique (Szilagyi et al., 2013; Ruiz-Cabello et al., 2015; Pavlovic et al., 2015).

Aggregation of solid particles determines the quality of many products by affecting the particle size distribution (PSD) and their morphology. The evolution of the PSD can be modelled using the population balance equations (PBEs) (Hulburt and Katz, 1964):

$$\frac{\partial f}{\partial t}+\sum_{i=1}^{3}\frac{\partial\left[v_i\left(\mathbf{x},t\right)f\right]}{\partial x_i}+\sum_{j=1}^{N}\frac{\partial\left(G_j f\right)}{\partial r_j}=B\left(\mathbf{x},\mathbf{r},t\right)-D\left(\mathbf{x},\mathbf{r},t\right) \tag{1}$$

where f denotes the density function of the dispersed phase properties distribution, v_i stands for the particle velocity in physical space described by coordinates x_i, G_j is the velocity of the particle in the space of dispersed phase properties (for example growth rate of crystals or dissolution rate of droplets), B and D denote the birth and death functions respectively.

To predict the behaviour of the system one has to express B and D functions by applying kernels suitable for specific processes and process conditions. The kernel depends on the fluid properties, the flow pattern and the particle properties.

Particles with the size smaller than 1 μm are called colloidal, whereas the larger ones — suspended (Elimelech et al., 1995). In this work the colloidal particles are considered.

Properties of particles in relation to the aggregation mechanism can be characterized using characteristic length and time scales of the flow field and the characteristic length and time scales characterising the particles. Resulting classification can be useful from the viewpoint of identification of relevant aggregation mechanism.

In case of particles that are subject to turbulent flow, a possible ranking of characteristic length scales can be based on the comparison of the particle size expressed by the particle radius a with the characteristic length scales for turbulence such as the Kolmogorov length microscale (Kolmogorov, 1941)

$$\lambda_k=\frac{\nu^{3/4}}{\varepsilon^{1/4}} \tag{2}$$

and the scale of the large, energy containing eddies, L (Hinze,1975)

$$L=\frac{\left(u'\right)^3}{\varepsilon} \tag{3}$$

where u' is the root-mean-square velocity fluctuation, ν denotes the fluid kinematic dynamic viscosity, ε is the rate of dissipation of the kinetic energy of turbulence per unit mass.

Particles of the radius a, smaller than the Kolmogorov length microscale, ($a<\lambda_k$), can be classified as small, and those of the size larger than the Kolmogorov microscale, ($a>\lambda_k$), large. In the group of large particles we have very large particles ($a>L$), aggregation of which is hardly possible in practice. For $\lambda_k<a<L$ inertial-convective effects control particle collisions.

To make analysis more complete, one should supplement the length-scale classification with the time-scale analysis. This can be done by comparing the time scales characterizing the flow: the Kolmogorov time microscale, τ_k and the Lagrangian integral time scale, T_L with the particle time scales.

The Kolmogorov time microscale characterises dynamics of small eddies (Kolmogorov, 1941)

$$\tau_k=\left(\frac{\nu}{\varepsilon}\right)^{1/2} \tag{4}$$

and the Lagrangian integral time scale, T_L, (Hinze, 1975) characterises dynamics of large ones

$$T_L=\beta\frac{\Lambda_f}{u'}=\frac{\beta(u')^2}{2\varepsilon}=0.2\,\frac{\left(u'\right)^2}{\varepsilon} \tag{5}$$

where Λ_f is the longitudinal integral scale of turbulence and $\beta\approx0.4$ is the constant of proportionality,

The characteristic time scales chacterising particles are: the diffusion time τ_D, and the relaxation time τ_p, respectively (Bałdyga and Krasiński, 2005):

$$\tau_D=\frac{\left(a_1+a_2\right)^2}{D_{12}^{\infty}} \tag{6}$$

$$\tau_p=\frac{16\rho_p\left(1+\frac{1}{2}\frac{\rho}{\rho_p}\right)a^2}{3\mu C_D Re_p} \tag{7}$$

where μ denotes the fluid dynamic viscosity, D_{12}^{∞} is the mutual Brownian diffusion coefficient of two particles, ρ_p and ρ are particle and fluid densities, C_D denotes the drag coefficient of the particle and Re_P is the particle Reynolds number.

In this work we consider aggregation of particles smaller than the Kolmogorov length microscale, having the relaxation time smaller than the Kolmogorov time microscale, for any value of the ratio of the Brownian diffusion time scale to the Kolmogorov time microscale. Namely, in the group of small particles we consider very small particles, for which $\tau_K\gg\tau_D$, or $a\ll\left(\frac{D_B^{\infty}\nu}{\varepsilon}\right)^{1/2}$ or whose Péclet number $Pe=\left(\frac{(\varepsilon/\nu)^{1/2}a^2}{D_B^{\infty}}\right)^{1/2}\ll1$, with their movements dominated by the Brownian motion, which leads to perikinetic collisions and perikinetic aggregation.

For $a<\lambda_k$ and $\tau_K\gg\tau_D$, or $a\gg\left(\frac{D_B^{\infty}\nu}{\varepsilon}\right)^{1/2}$, so for the Péclet number $Pe=\left(\frac{(\varepsilon/\nu)^{1/2}a^2}{D_B^{\infty}}\right)^{1/2}\gg1$, we consider particle movements that are induced by the fluid deformation, which leads to orthokinetic collisions and orthokinetic aggregation.

This means that a basic aggregation kernel can be determined by solving the convection–diffusion equation for the pair probability function of the solid particles present in the DLVO potential field for sub-Kolmogorov scale flow structure including the whole range of Pe values. An approach presented by Melis et al. (1999) is applied here with extensions including particles of unequal size, hydrophobic attractions (Mishchuk, 2011) and particle/particle as well as particle/bubble interactions (Usui and Barouch, 1990). Although this method of kernel derivation is precise there are difficulties to apply it to simulations with the PBEs and CFD models because it would require solving a partial differential equation in each grid cell, in every iteration and for each time step. For such applications one can use a computationally less expensive method. In the present work we propose an aggregation kernel based on the modified Fuchs stability ratio approach. The modified stability ratio has been derived using a concept of small scale turbulent diffusion that competes with particle convection generated by repulsion forces and fluid deformation.

The aggregation rate constants obtained using the simplified method are compared to the predictions of the full model based on convection–diffusion approach, and to prediction of other simplified model (Bałdyga and Orciuch, 2001). Proposed approach leads to better prediction of the aggregation kernel for strong electrostatic repulsion between particles.

2. The full convection–diffusion equation approach

In a turbulent flow of a solid suspension, particles smaller than the Kolmogorov microscale are surrounded by the extensional flow field of the fluid (Batchelor and Green, 1972). The fluid velocities in radial and tangential directions are given by:

$$v_{f,r}=\frac{1}{2}\langle E\rangle\bar{a}\xi\left[1-A\left(\xi,\lambda\right)\right]\left(3\cos^2\theta-1\right) \tag{8}$$