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Simulating orthokinetic heterocoagulation and cluster growth in destabilizing suspensions

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ABSTRACT

Using direct numerical simulation, we investigate the coagulation behavior of non-Brownian colloidal particles as exemplified by Al_2O_3 particles. This yields the so-called capture efficiency, for which we give an analytical expression, as well as other time-dependent variables such as the cluster growth rate. Instead of neglecting or strongly approximating the hydrodynamic interactions between particles, we include hydrodynamic and non-hydrodynamic interactions in a Stokesian dynamics approach and a comprehensive modeling of the interparticle forces. The resulting parallelized simulation framework enables us to investigate the dynamics of polydisperse particle systems composed of several hundred particles at the same high level of modeling we used for a close investigation of the coagulation behavior of two unequal particles in shear flow. Appropriate cluster detection yields all the information about large destabilizing systems, which is needed for models used in flow-sheet simulations. After non-dimensionalization, the results can be generalized and applied to other systems tending to secondary coagulation.

Introduction

Destabilization of suspensions in shear flow and during sedimentation are important topics in all kinds of suspension-related engineering, such as chemical engineering, process engineering, civil engineering, and wastewater treatment. Numerical simulation is a valued means in investigating the fundamental mechanisms during destabilization, and for the design of coagulation-related processes, i.e., aggregation, agglomeration, and flocculation. With progress in modeling, code parallelization, and access to supercomputers, increasingly complex systems can be simulated within an acceptable time span. Nevertheless, the larger and the more complex a simulated system is, the more modeling has to be performed. Modeling based on the population balance equation (PBE) are appropriate in simulating coagulation-related processes on an industrial scale (Gerstlauer, Gahn, Zhou, Rauls, & Schreiber, 2006). They are mainly applied to investigate and predict aggregation and agglomeration in stirred tank vessels (Hollander, Derksen, Portela, & Vanden Akker, 2001), but can also be applied to complex solid–liquid separation processes, such as the settling of activated sludge in a secondary clarifier (Torfs, Dutta, & Nopens, 2012). PBE models heavily rely on coagulation and breakup kernels, which give the probability of coagulation and breakup of aggregates, agglomerates or flocs. If the model used does not describe well the physics of the considered system, the prediction from such a simulation is rather poor (Torfs et al., 2012). Apart from giving a better understanding of the underlying physics, direct numerical simulations can provide the models for strongly model-based simulations, such as PBE, but also for analytic models used in flow-sheet simulations. There are numerous studies dealing with the simulation of agglomerate and aggregate breakup and deformation (Conchuir, Harshe, Lattuada, & Zaccone, 2014; Dosta, Antonyuk, & Heinrich, 2013; Harshe & Lattuada, 2012; Higashitani, Iimura, & Sanda, 2001; Manounou & Rémond, 2014; Seto, Botet, Auernhammer, & Briesen, 2012; Zeidan, Xu, Jia, & Williams, 2007), as well as several studies considering the modeling and simulation of coagulation (Curtis & Hocking, 1970; Feke & Schowalter, 1983; Smoluchowski, 1917; Van de Ven & Mason, 1976), but only a limited number of studies considering coagulation and settling at the same time (Davis, 1984; Han & Lawler, 1991; Qiao, Li, & Wen, 1998). Work in the field of modeling and prediction of the coagulation probability can be classified according to the level of approximation (Khadilkar, Rozelle, & Pisupati, 2014), as well as by the type of coagulation

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investigated, differentiated as either perikinetic, orthokinetic or differential settling coagulation. Perikinetic coagulation is mainly driven by Brownian motion and orthokinetic coagulation by flow. This means mostly shear flow, but depending on the definition it can also include settling (Somasundaran, 2006). Coagulation due to differential settling is coagulation owing to the fact that in general a larger or denser particle settles faster than a smaller or lighter particle. Technically speaking, this effect differs from flow-driven coagulation, as here the driving force is a volume force and not a hydrodynamic force, which is a surface force. A distinction by the Peclet number nonetheless yields only two groups: inertia-dominated coagulation and Brownian motion-dominated coagulation. Of course, there is a transition regime and on a technical scale coagulation due to flow and that due to differential settling are almost always superimposed. Therefore, we leave the distinction to the reader to decide as further discussion is beyond the scope of this work. Here we concentrate on non-Brownian coagulation and refer to it as orthokinetic coagulation.

A classical way to predict orthokinetic coagulation in suspensions is the consideration of two particles in a simple shear flow, from which a derivation of the so-called orthokinetic collision rate is possible. This can be done for example based on conditional pair distribution functions (usually done if Brownian motion plays a role); see for example Feke and Schowalter (1983) and Qiao et al. (1998), or by a direct investigation of the trajectories of two intercepting particles. In his famous work, Smoluchowski (1917) determined the collision rate of colloidal particles based on simple assumptions, among them being that hydrodynamic interactions are negligible and that around each particle there is a sphere of attraction wherein two particles coagulate instantly when their spheres overlap. Nevertheless, the resulting collision rates are remarkably good and are in various forms widely used. Usually these collision rates are modified by a capture efficiency, which is defined as the ratio of the observed collision rate to the collision rate proposed by Smoluchowski (Van de Ven & Mason, 1977). There are numerous studies using a two-particle approach in bispherical coordinates to obtain the capture efficiency for two spheres in a simple shear flow (Adler, 1981; Balakin, Hoffmann, & Kosinski, 2012; Kobayashi, 2008; Lin et al., 2006; Sato, Kobayashi, & Adachi, 2004; Van de Ven & Mason, 1977; Vanni & Baldi, 2002; Wang, 1992). The resulting orthokinetic capture efficiency can be applied to compute the collision rate used in PBE simulations. Nevertheless, the applicability of simulations using bispherical coordinates is limited to a consideration of only two particles.

Using a meshfree simulation approach for hydrodynamic interactions between particles (Brady & Bossis, 1988; Durlofsky, Brady, & Bossis, 1987) and detailed modelling of other effects occurring, such as lubrication (Davis, Serayssol, & Hinch, 1986) and interparticle interactions covered by Derjaguin–Landau–Verwey–Overbeek (DLVO) theory (Feke, Prabhu, Mann, & Iii, 1984; Verwey & Overbeek, 1999), permits a close investigation of the coagulation behavior of two particles as well as studies on destabilization of particle systems with a large number of settling particles (Bülow, Hamberger, Nirschl, & Dörfler, 2014; Bülow, Nirschl, & Dörfler, 2015). In this work, we show that both ways yield results for the coagulation probability, the collision rate and the cluster growth rate, which are essentials for large-scale simulations using PBE and simplified methods such as flow-sheet simulations.

The structure of this paper is as follows: first we give a quick overview of the method we used to simulate the behavior of suspensions, and we present the models used for particle–particle interactions. We focus on a new model for lubrication forces between particles at almost-contact. The results obtained from numerical investigations in the binary orthokinetic heterocoagulation of Al_2O_3 particles in shear flow lead to a convenient analytical expression for the orthokinetic capture efficiency. Furthermore, we show how to reduce the effort needed in doing similar numerical experiments. We conclude this work by giving results from a cluster detection applied to simulation data from numerical experiments on destabilizing systems of suspended particles. In addition to a comprehensive insight into the process, this procedure yields useful data such as cluster growth rates and other information needed for flow-sheet simulations.

Methods

Underlying equations for the particle motion

We consider the motion of N particles for which the effects of interparticle forces and hydrodynamics are dominant and those of Brownian motion are negligible. If these particles settle in an otherwise undisturbed fluid or are exposed to a simple shear flow with low to moderate shear rate $\dot{\gamma}$ such that a vanishing Reynolds number can be assumed, the quasi-steady Stokes equations can describe the fluid motion appropriately. The translational motion of a spherical particle α suspended in a fluid can generally be described by the dimensionless Langevin equation (Brady & Bossis, 1988; Ichiki & Hayakawa, 1995),

$$St\left(\frac{a_\alpha}{L_0}\right)^3 \frac{d}{dt}\boldsymbol{U}_\mathrm{p} = \boldsymbol{F}_\alpha^\mathrm{h} - \left(\frac{a_\alpha}{L_0}\right)^3 \boldsymbol{e}_z + \boldsymbol{F}_\alpha^{\mathrm{i,St}} + \frac{1}{Pe}\boldsymbol{F}_\alpha^{\mathrm{i,Pe}}, \tag{1}$$

with the Stokes number St defined as the Reynolds number Re scaled by the mass density ratio,

$$St = \frac{2}{9}\frac{\rho_\mathrm{p}}{\rho_\mathrm{f}} Re, \tag{2}$$

and the vector $\mathbf{e}_z \in \mathbb{R}^3$ pointing in the positive z-direction (without loss of generality, the applied centrifugal force points in the negative z-direction). The dimensionless angular momentum balance is given by,

$$St\frac{2}{5}\left(\frac{a_\alpha}{L_0}\right)^5 \frac{d}{dt}\boldsymbol{\omega}_\mathrm{p} = \boldsymbol{T}_\alpha^\mathrm{h} + \boldsymbol{T}_\alpha^{\mathrm{i,St}} + \frac{1}{Pe}\boldsymbol{T}_\alpha^{\mathrm{i,Pe}}. \tag{3}$$

In Eqs. (1) and (3), $\mathbf{U}_\mathrm{p} \in \mathbb{R}^3$ is the translational velocity of particle α, $\mathbf{F}_\alpha^\mathrm{h} \in \mathbb{R}^3$ the hydrodynamic force acting on the particle, $\mathbf{F}_\alpha^{\mathrm{i,St}} \in \mathbb{R}^3$ interparticle forces of the same scale as $\mathbf{F}_\alpha^\mathrm{h}$, and $\mathbf{F}_\alpha^{\mathrm{i,Pe}} \in \mathbb{R}^3$ interparticle forces which need to be scaled by the Peclet number Pe. Also $\boldsymbol{\omega}_\mathrm{p} \in \mathbb{R}^3$ denotes the angular velocity of particle α, $\mathbf{T}_\alpha^\mathrm{h} \in \mathbb{R}^3$ the hydrodynamic torque acting on the particle, and $\mathbf{T}_\alpha^{\mathrm{i,St}} \in \mathbb{R}^3$ and $\mathbf{F}_\alpha^{\mathrm{i,Pe}} \in \mathbb{R}^3$ are torques corresponding to the respective forces. Assuming a constant particle mass density ρ_p, the mass m_α of a spherical particle α is $m_\alpha = \frac{4}{3}\pi\rho_\mathrm{p}a_\alpha^3$, with particle radius a_α. With the same assumption, the moment of inertia tensor $\mathbf{I}_\alpha \in \mathbb{R}^{3\times3}$ takes the form $\mathbf{I}_\alpha = \frac{8}{15}\pi\rho_\mathrm{p}a_\alpha^5\mathbf{I}d$, with $\mathbf{I}d$ the 3×3 identity matrix. For nondimensionalization, we used the characteristic length L_0, characteristic force scale $F_0 = 6\pi\mu_\mathrm{f}L_0U_0$, and characteristic velocity U_0, the Stokes velocity of a particle of radius L_0 in the applied centrifugal field.

The dimensionless Eqs. (1) and (3) contain two dimensionless numbers, St and Pe. The Stokes number St of a monodisperse system of spherical particles, i.e., for $a_\alpha = L_0 \forall \alpha \in [1, N]$, is given in Eq. (2). For a polydisperse system, with L_0 chosen as the mean value of the particle radius distribution, one can define a Stokes number specific to a particle α,

$$St_\alpha = \left(\frac{a_\alpha}{L_0}\right)^3 St = \left(\frac{a_\alpha}{L_0}\right)^3 \frac{2}{9}\frac{\rho_\mathrm{p}}{\rho_\mathrm{f}} Re = \frac{m_\alpha U_0^2}{6\pi\mu_\mathrm{f}L_0^2U_0},$$

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