Advanced Powder Technology 26 (2015) 705–710

Contents lists available at ScienceDirect

Advanced Powder Technology

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

Original Research Paper

Stability of restructured non-fractal aggregates in simple shear flow

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ARTICLE INFO

Article history:
Received 22 September 2014
Received in revised form 25 November 2014
Accepted 11 December 2014
Available online 24 December 2014

Keywords:
Aggregate
Restructuring
Stokesian dynamics
Coordination number

ABSTRACT

The restructuring behavior of non-fractal aggregates in simple shear flow is numerically investigated. The change in internal structure of aggregates having different packing properties is examined by Lagrangian simulation method. The many-body hydrodynamic interaction is rigorously estimated by Stokesian dynamics approach while the adhesion of aggregate is manifested via particle–particle interaction. The simulation results show that the restructuring of aggregate originates from the superimposition of rotational and extensional component of simple shear flow. The aggregate rearranges its particles so that a stable structure corresponding to the applied shear flow is obtained. The stable structure is considered as dynamic equilibrium resulting from the balance of the forming and the disintegrating of the bonds between particles. The stable structure of aggregate is dependent strongly on shear condition but weakly on initial structure of aggregate. Despite of the significant difference in the initial packing properties, the stable structure reveals only slightly different. The dependence of stable structure on high shear tress condition is similar for all aggregates. The difference in stable structure of aggregate at low shear stress arises from the irreversible behavior of particle from quasi-stable structure to static structure.

1. Introduction

The aggregation and dispersion processes of colloidal particles are widely seen in various engineering fields such as environmental engineering, material engineering, to name a few. Understanding the behavior of colloidal aggregates in fluid flow is one of the fundamental issues for the prediction and control of the dispersion state of suspension. Population balance model has been developed for quantitative prediction of the size distribution of aggregates from the parent aggregates. In this model, the important parameters on the aggregation and breakup of aggregate are required [1]. Simulation and experimental studies have found that the behaviors of aggregate in flow field, including rigid body, restructuring and breakup, are dependent on the hydrodynamics stress and the strength of aggregate [2–5]. In addition, it is well-known that the aggregate has a wide variety of structures, and the hydrodynamic properties of the aggregates greatly depend on these structures. When the restructuring occurs, the aggregate behaves complexly because the particle-fluid interaction is complicated while the dynamic system has to be taken into account.

Many researchers examined the behavior of aggregate relying on the change in the space-filling properties i.e. fractal dimension. They found that in shear flow, the aggregates tended to have high fractal dimension by means of experiment [1], numerical simulation [6] and analytical model [7]. Further studies showed that the breakup behavior of the high fractal dimension aggregate was significantly diverse [4,7–9]. One of the reason is that the aggregate with high space-filling properties may have the connectivity of the particle vary, leading to different ways in force distribution and propagation. Moreover, Harada et al. [4] found out that the breakup behavior of non-fractal aggregate (i.e. fractal dimension equals 3) was much more complicated because the aggregate continuously restructured before the breakup. The importance of restructuring has also been reported via the kinetic models of aggregation and dispersion [10,11]. Although the restructuring of aggregate is critical to the breakup process, little understanding on the restructuring is revealed, even in the case of isolated aggregate.

There have only been a few studies on the restructuring dynamics of aggregate in shear flow. Experimental studies such as Blaser [3] confirmed the change in aggregate's structure when the shear was applied. Numerical researches reported that the fractal aggregate restructured and became more dense in terms of volume fraction [12] and radius of gyration [5] for low shear rate. Though the two aforementioned parameters are commonly used to evaluate the compactness and the size of the aggregate, they are quite sensitive to the shape of aggregate [12] and somewhat inappropriate

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http://dx.doi.org/10.1016/j.apt.2014.12.009

to describe the internal structure. Additionally, the connectivity of non-fractal aggregate becomes more complex during restructuring [4]. Harada et al. [13] showed that the restructuring of dense particle cluster included three stages: firstly the aggregate rearranged to a structure corresponding to shear stress, then the cracks grew inside the aggregate for a long time, finally aggregate irregularly changed toward rupture.

The aim of this study is to understand the restructuring behavior of non-fractal aggregates before breakup in simple shear flow by Lagrangian simulation. Since our interest focus on the effect of surrounding flow on the particles, we employ Stokesian dynamics for the calculation of hydrodynamic interaction. The restructuring process of aggregate with different connectivity is performed under various shear flow conditions. We evaluate the restructuring by examining the change in internal structure of the aggregate dynamically. Detail of the effect of the connectivity and flow conditions on the restructuring of aggregate is discussed.

2. Simulation method

The full description of the simulation method can be found in the previous studies [4,13]. Here we summarize the essential governing equations, which involve the hydrodynamic interaction of multiple primary particles composing the aggregate. The motion of the rigid and spherical particles is simulated by Stokesian dynamics approach [14]. The relation between force, torque, stresslet exerting on particles, and the motion of particles relative to the imposed flow is given in Eq. (1).

$$\begin{pmatrix} \boldsymbol{F} \\ \boldsymbol{T} \\ \boldsymbol{S} \end{pmatrix} = \overline{\boldsymbol{R}} \cdot \begin{pmatrix} \boldsymbol{U} - \boldsymbol{u}^{\infty} \\ \boldsymbol{\Omega} - \boldsymbol{\Omega}^{\infty} \\ -\boldsymbol{E}^{\infty} \end{pmatrix} \tag{1}$$

where $\boldsymbol{F}, \boldsymbol{T}, \boldsymbol{S}$ are the external force, torque and stresslet acting on particles; $\boldsymbol{U}, \boldsymbol{\Omega}$ the particle translational velocity and rotational velocity; $\boldsymbol{u}^{\infty}, \boldsymbol{\Omega}^{\infty}, \boldsymbol{E}^{\infty}$ the flow velocity, rotational velocity and rate of strain tensor, $\overline{\boldsymbol{R}}$ the grand resistance matrix which is dependent only on the position of the particles. Readers can refer to articles [15–17] for details on the method and calculation of the grand resistance matrix. From Eq. (1), the translational and rotational velocity of particles with prescribed forces and torques are given as follows:

$$\begin{pmatrix} \boldsymbol{U} \\ \boldsymbol{\Omega} \end{pmatrix} = \begin{pmatrix} \boldsymbol{U}^{\infty} \\ \boldsymbol{\Omega}^{\infty} \end{pmatrix} + \begin{pmatrix} \overline{\boldsymbol{R}}_{FU} & \overline{\boldsymbol{R}}_{F\Omega} \\ \overline{\boldsymbol{R}}_{TU} & \overline{\boldsymbol{R}}_{T\Omega} \end{pmatrix}^{-1} \cdot \left[\begin{pmatrix} \boldsymbol{F} \\ \boldsymbol{T} \end{pmatrix} + \begin{pmatrix} \overline{\boldsymbol{R}}_{FE} \\ \overline{\boldsymbol{R}}_{TE} \end{pmatrix} : \boldsymbol{E}^{\infty} \right] \tag{2}$$

where $\overline{\boldsymbol{R}}_{FU}, \overline{\boldsymbol{R}}_{F\Omega}$, etc. are the components of the grand resistance matrix $\overline{\boldsymbol{R}}$. The instantaneous position of all particles is calculated by updating the matrices in Eq. (2) with each time step.

Regarding the simple shear flow characterized by shear rate $\dot{\gamma}$, the surrounding flow field $\boldsymbol{u}^{\infty}, \boldsymbol{\Omega}^{\infty}$ and $\boldsymbol{E}^{\infty}$ are described respectively below.

$$\boldsymbol{u}^{\infty}(\boldsymbol{r}) = \boldsymbol{\Omega}^{\infty} \times \boldsymbol{r} + \boldsymbol{E}^{\infty} \cdot \boldsymbol{r} \tag{3}$$

$$\boldsymbol{\Omega}^{\infty} = -\frac{\dot{\gamma}}{2} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad \boldsymbol{E}^{\infty} = \frac{\dot{\gamma}}{2} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{4}$$

Fig. 1 shows the coordinate system of our calculation and the initial configuration of some non-fractal aggregates. The aggregate is composed of one hundred primary particles. The particles are assumed smooth and spherical with a diameter of $2a = 650$ nm. The properties of particles and fluid are those of polystyrene and ethanol. The particle density, the fluid density and the fluid viscosity are $\rho_p = 1056\ \mathrm{kg/m^3}$, $\rho_f = 790\ \mathrm{kg/m^3}$ and $\mu = 1.2 \times 10^{-3}$ Pa s, respectively. The particle–particle interaction is calculated from

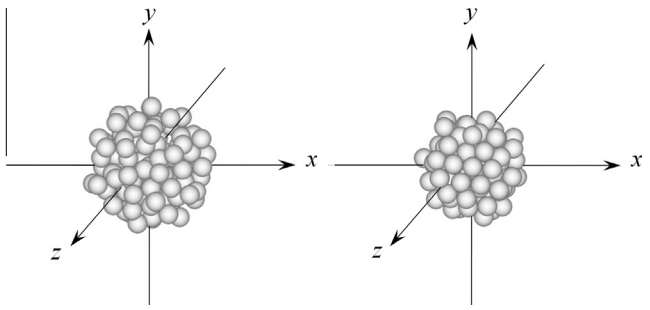

Fig. 1. The coordinate system and initial configurations of aggregates $k_0 = 2.00$ (left) and $k_0 = 5.54$ (right).

the attractive London-van der Waals potential [18,19]. As the particles approach very close at a few Angstrom, the attractive force is no longer dominant because the other complex phenomena at molecular scale govern the interaction [20]. For this reason, we simply set the attractive force to be zero when the distance of particle's surface is less than 1 nm. The overlapping of particles is prevented due to the lubrication effect included in the grand resistance matrix [14,15]. Because of the discretization of the simulation, we choose appropriately small time step for each simulation condition to assure that the particles definitely do not overlap. It should be notice that there are some works on the restructuring and breakup of aggregate considering more complex particle interactions such as tangential force when the particles are in contact [1,6,12,21]. Though the particle–particle interaction used in our method is simple, we verify that some parameters, which express the behaviors of the aggregate, are relatively in agreement with either experiment study [3] or simulation study employing more complex contact force [6,21]. Therefore, the contact force is neglected for the sake of simplicity. In this study, the properties of particle and fluid is appropriately chosen so that the effect of fluid inertia, particle inertia and Brownian motion of particle is neglected due to small Reynolds number, Stokes number and large Péclet number. The detailed discussion on the assumptions, calculation conditions and verification of the simulation are described in the articles [4,13].

The aggregate shown in Fig. 1 is created by employing particle-cluster aggregation model to randomly distributed particles to which an assumed centripetal force is applied. By this method, the isotropy of the particles is obtained in the case that the aggregate is large enough to neglect the effect of surface particles [22]. The non-fractal property of the aggregate is exhibited via its spherical morphology as can be seen in the figure. The connectivity of aggregate is expressed by coordination number which has been widely investigated as an important packing property of granular media at a local scale [23]. Coordination number is defined as the average number of particle adjacent to a particular one within designated separation of particle's surface. The chosen separation has to satisfy to describe the attraction forces among particles. We calculate the coordination number by counting the number of particle if the surface distance of two particles is less than 2 nm. We verify that the coordination number is not considerably influenced if the surface distance varies within a few nm. Different from the fractal aggregate, the non-fractal aggregate may have its internal connectivity vary. Therefore, the non-fractal aggregate used in the study has different initial structures from loose to dense, equivalent to the initial average coordination number from 2.00 to 5.54. The aggregates at these extreme conditions are given in Fig. 1. The most dense aggregate has the coordination number $k_0 = 5.54$ somewhat smaller than that of random closed-packed particles around 5.9–8.5 [24–26]. This is because the number of particle of the aggregate is only one hundred, much smaller than the one that used in the literature from thousands to ten thousands