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Original Research Paper

Restructuring capability of non-fractal aggregate in simple shear flow

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ABSTRACT

A unique pattern interpreting the restructuring of non-fractal aggregate is established. The restructuring of an aggregate from initial structure toward a stable structure is well presented by a linear relation between the saturation degree of particle connection, and the inversed strength of aggregate. The dynamics of restructuring for different initial configuration of aggregate, from very loose to dense, in various simple shear flow condition is numerically performed. The temporal change in properties of aggregate is analyzed in terms of coordination number and volume fraction. The simulation employs Stokesian dynamics for the estimation of many-particle hydrodynamic interaction while the particle–particle interaction is calculated by van der Waals potential. Simulation results show that the aggregate restructures and exists in a stable state corresponding to the shear flow condition. The transition among the stable aggregates somewhat expresses reversible behavior. Especially in weak flow, the aggregate gradually reaches its limit structure whose properties such as coordination number and volume fraction are typically determined. Such limit aggregate plays an important role for predicting the restructuring of any non-fractal aggregate in any fluid condition. Moreover, the penetration effect of fluid flow on aggregate is discussed by means of porous sphere model.

1. Introduction

The behavior of colloidal aggregate in fluid flow is fundamentally important for the prediction and control of dispersion of particles. In general, the behavior of aggregate in flow field, such as rigid-like motion, restructuring and breakup, depends on the hydrodynamic stress acting on the aggregate, and the strength of aggregate itself [1–5]. The task of determining such hydrodynamic stress and strength of aggregate is very complicated since the colloidal aggregate has a wide variety of structure which greatly affects those properties. The restructuring of aggregate, where the primary particles of the aggregate are relatively in motion but still attach together, can be considered as an intermediate stage between the rigid-like motion and breakup. While the breakup of aggregate is well established by extensive studies [1,2,4–9], the restructuring has not been properly understood. The restructuring of aggregate has significant impact on the breakup and aggregation of aggregate [10,11] because it possibly occurs either before [4,8] or after the breakup event [6,9]. As a result, the structure of aggregate and, consequently, the rheological properties of the colloidal suspension are completely affected.

The behavior of aggregate in simple shear flow has attracted a lot of interest due to its ubiquity in engineering fields. Fractal dimension, which can be interpreted as a space-filling property, is often used to characterize the structure of particle aggregates. In non-sheared system, the aggregate often has ramified structures whose fractal dimension is low. In sheared system, the aggregate appears more compact and is apt to exist in the form of high fractal dimension, which is demonstrated by experiment [1], simulation [6,9,12], and analytical model [13]. One of the possible reasons is that the restructuring of the aggregate has occurred, the branches of the aggregate bends and reconnects, leading to a more compact structure [4,5,14]. Furthermore, the breakup of the high fractal dimension aggregate behaves diversely whereas that of the low fractal dimension aggregate is predictable [4,15]. Explanation for the former can be analyzed from two perspectives. From the static point of view, the complex connectivity inside the high fractal aggregate influences the way of distribution and propagation of force, therefore the resulting stress differs within parts of the aggregate [15,16]. From the dynamic point of view, the restructuring of aggregate occurs, leads to significant change in aggregate's structure compared to its initial configuration, and eventually determines the way that the aggregate breaks [4,17,18]. Therefore, understanding the restructuring behavior of high fractal dimension aggregate contributes important information for kinetics of

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aggregation model and breakup model. The aggregates at upper limit of fractal dimension, $d_f = 2.0$ for two-dimensional or $d_f = 3.0$ for three-dimensional aggregate, are dense and radial-density independent structures [16]. In the scope of this study, we define such aggregate as non-fractal aggregate to emphasize the difference of its structure compared to the fractal and ramified aggregate. Experimental study for two-dimensional non-fractal aggregate shows that there is a significant change in the internal structure of aggregate: under shear flow, the particles of the aggregate rearrange into a more ordered structure [19]. For three-dimensional aggregate [1], the change of internal structure of aggregate is unknown due to lack of proper observing devices. We have conducted numerical simulation to study about the restructuring behavior of non-fractal aggregate in the previous work [20]. We have found that in simple shear flow, the non-fractal aggregate restructures via change in internal connectivity so that a more stable structure is obtained. Such stable structure has similar appearance but notable difference in internal connectivity compared to the initial structure. A kinetic model represents change in coordination number of aggregate is proposed.

The content of this article shows succeeding output of our previous study [20]. The previous article focuses on the existence of stable aggregate during the restructuring, and the dependence of the internal connectivity of aggregate on the condition of fluid flow as well as the initial aggregate. In this article, we attempt to establish a comprehensive approach to predict the corresponding structure of a given aggregate in simple shear flow by considering the physical interpretation of the restructuring in terms of the capacity of making particle connection and the strength of aggregate. In detail, investigations for the uniqueness of stable aggregate, the limit of restructuring, the governing properties that decide the structure of aggregate, and the role of hydrodynamic stress, are carried out. The dynamics of restructuring behavior of non-fractal aggregates before breakup in simple shear flow is performed by Lagrangian simulation approach. The many-body hydrodynamic interaction among the identical particles composing the aggregate is estimated by Stokesian dynamics. The restructuring of non-fractal aggregate with different initial configuration is examined under various fluid shear flow conditions.

2. Simulation method

The simulation method is almost similar to our previous study [20]. For convenience, we emphasize the concept, governing equations and simulation conditions of the study. The basis of our simulation method for the hydrodynamic interaction of multiple particles in fluid flow is Stokesian dynamics [21,22]. The content of the lengthy and complicated Stokesian dynamics can be found in the work of Durlofsky et al. [22] and the references therein. The FTS version of Stokesian dynamics is used to study the motion of particles in an imposed flow. In summary, when the particle is in relative motion to the fluid flow, the particle exerts force $\boldsymbol{F}_H$ and torque $\boldsymbol{T}_H$ on fluid. In opposite, fluid exerts on particle the hydrodynamic force $-\boldsymbol{F}_H$, torque $-\boldsymbol{T}_H$, and stresslet S. For a particle with hydrodynamic interaction $-\boldsymbol{F}_H$, $-\boldsymbol{T}_H$ and non-hydrodynamic interaction $\boldsymbol{F}$, $\boldsymbol{T}$, the neglect of particle inertia leads to $\boldsymbol{F}_H \approx \boldsymbol{F}$ and $\boldsymbol{T}_H \approx \boldsymbol{T}$. Finally, for a finite number of particles in fluid flow, the relation between the force exerting on particles and the relative motion of particles to the fluid flow is shown as following

$$\begin{pmatrix} \boldsymbol{F} \\ \boldsymbol{T} \\ \boldsymbol{S} \end{pmatrix} = \boldsymbol{M}^{-1} \cdot \begin{pmatrix} \boldsymbol{U} - \boldsymbol{u}^{\infty} \\ \boldsymbol{\Omega} - \boldsymbol{\Omega}^{\infty} \\ -\boldsymbol{E}^{\infty} \end{pmatrix}, \boldsymbol{M}^{-1} = \begin{pmatrix} \boldsymbol{R}_{FU} & \boldsymbol{R}_{F\Omega} & \boldsymbol{R}_{FE} \\ \boldsymbol{R}_{TU} & \boldsymbol{R}_{T\Omega} & \boldsymbol{R}_{TE} \\ \boldsymbol{R}_{SU} & \boldsymbol{R}_{S\Omega} & \boldsymbol{R}_{SE} \end{pmatrix} \tag{1}$$

where $\boldsymbol{U}, \boldsymbol{\Omega}$ is the particle velocity and rotational velocity; $\boldsymbol{u}^{\infty}, \boldsymbol{\Omega}^{\infty}, \boldsymbol{E}^{\infty}$ the velocity, rotational velocity and rate of strain tensor of the undisturbed flow; $\boldsymbol{R}_{FU}, \boldsymbol{R}_{TU}$, etc. the components of the resistance matrix which are determined from the mobility matrix $\boldsymbol{M}$ and dependent only on the position of the particles. The calculation method of the mobility matrix $\boldsymbol{M}$ can be found in Durlofsky et al. [22]. According to Eq. (1), the translational and rotational velocity of particles is calculated as below

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

where $\overline{\boldsymbol{R}}_{FU}, \overline{\boldsymbol{R}}_{F\Omega}$, etc. are the components of the grand resistance matrix $\overline{\boldsymbol{R}}$ in which the lubrication correction is included by the following form

$$\overline{\boldsymbol{R}} = \boldsymbol{M}^{-1} - \boldsymbol{M}_{2B}^{-1} + \boldsymbol{R}_{2B} \tag{3}$$

where $\boldsymbol{M}_{2B}$ is the two-body mobility matrix calculated in a similar way with $\boldsymbol{M}$, $\boldsymbol{R}_{2B}$ the two-body resistance matrix [22–24]. The dynamic behavior of all particles is performed by numerical integration of Eq. (2) while the matrices are continuously updated with each time step.

The behavior of an isolated aggregate is investigated in simple shear flow characterized by shear rate $\dot{\gamma}$. The undisturbed flow $\boldsymbol{u}^{\infty} = (\dot{\gamma} y, 0, 0)^T$ in Cartesian coordinates, which is viably used in Eq. (2), is described as

$$\boldsymbol{u}^{\infty}(\boldsymbol{r}) = \boldsymbol{\Omega}^{\infty} \times \boldsymbol{r} + \boldsymbol{E}^{\infty} \cdot \boldsymbol{r} \tag{4}$$

$$\boldsymbol{\Omega}^{\infty} = -\frac{\dot{\gamma}}{2} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad \boldsymbol{E}^{\infty} = \frac{\dot{\gamma}}{2} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{5}$$

The simulation condition is similar to our previous study [20]; the summary can be found in Table 1. The interaction between the hard-sphere particles is estimated by retarded van der Waals potential based on Hamaker geometrical factor and Lifshitz theory. The complicated formulae for the renowned potential are completely given in the relevant articles [25,26]. Additionally, when the surface distance of particles is less than a cutoff distance of 1 nm, the attractive force is simply set zero since the other complex phenomena at molecular scale may be dominant and should be taken into account [27]. The overlap of particles does not occur due to the lubrication correction and suitably small time-step. Recently, researches on the behavior of aggregate sometimes involve more complicated interparticle interaction, e.g. tangential force, due to its significant effect on the restructuring fractal aggregate [5,6,14]. In particular, it is reported that the branches of the fractal aggregate is more invulnerable to bending moment [5,6,28]. However, a systematic understanding on such tangential force has not been well established yet, leading to difficulties and uncertainties in constructing models. Our simulation with the prescribed force in this study is simple but able to represent an example of particle aggregates with central force, and the scope of our study is to examine the effect of hydrodynamics of many-body rather than the effect of interparticle interaction on the aggregate.

Table 1
Basic simulation conditions.

Parameter	Value
Number of particle of aggregate	$N = 100$
Particle radius	$a = 325$ nm
Particle density	$\rho_p = 1056$ kg/m^3
Fluid density	$\rho_f = 790$ kg/m^3
Fluid viscosity	$\mu = 1.2 \times 10^{-3}$ Pa s
Non-retarded Hamaker constant (for the condition of this study)	$A_H = 9.68 \times 10^{-21}$ J
Cut-off distance	$\delta = 1$ nm