学 位 論 文 内 容 の 要 旨

DISSERTATION ABSTRACT

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Numerical simulation of restructuring behavior of non-fractal aggregate in simple shear flow

(一様せん断流中における非フラクタル凝集体の再配列的挙動に関する数値シミュレーション)

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 colloidal suspension, which is widely encountered in engineering fields, especially when high accuracy is required. The structure of the aggregate has a significant role for either the microstructure or macroproperties of the suspension. In fluid flow, the restructuring of aggregate can occur before and after the breakup, which contributes significant affect to the overall performance of the suspension. It is found that in fluid flow, the aggregate restructures and often exists at high fractal dimension structure, and the behavior of such aggregates complicatedly varies. Understanding the internal structure of an aggregate during restructuring is important for developing highly accurate model predicting the properties of suspension. Therefore, the restructuring behavior of non-fractal aggregate in simple shear flow is numerically investigated.

In this study, the change in internal structure of an isolated non-fractal aggregate in simple shear is examined by Lagrangian simulation method. The aggregate is composed of a number of mono-sized, spherical, and hard particles. The attraction between particles is calculated by the retarded van der Waals interaction, which is estimated by Lifshitz theory and Hamaker geometrical factors. The very complex many-body hydrodynamic interaction is rigorously determined by Stokesian dynamics approach. The aggregate with different packing structure, from very loose to dense as random-close packing, in various shear flow conditions is dynamically investigated.

First of all, the extent of restructuring regarding the fluid flow, initial structure of aggregate, and the progressing time is inspected. The change in internal structure of the non-fractal aggregate in terms of coordination number is examined. Typically, after subjected to shear flow, the aggregate rotates around the vorticity axis and deforms along the streamline. The deformation progresses with time: from spherical shape to ellipsoidal one; finally followed by recovering to almost spherical shape. Simultaneously, the coordination number of aggregate alters and reaches a stable value. The restructuring of aggregate originates from the superimposition of rotational and extensional component of simple shear flow. The aggregate restructure so that a stable structure corresponding to the applied shear flow is obtained. At the same fluid shear stress condition, despite of the significant difference in the initial packing properties, the stable structure of aggregate likely exist at quite compact state, and the stable structure reveals only slight difference. The dependence of stable structure on fluid shear stress condition shows similar manner for all aggregates. The stable aggregate in weaker flow is more dense than that in the stronger flow. However there is a limit for such compact structure. The stable structure is considered as dy-

namic equilibrium resulting from the balance of the forming and the disintegrating of links between particles.

The next task is to determine a general relation of the stable aggregate in shear flow. The transition among stable aggregates is found to have some reversibility. Further analysis on the stable aggregate at the limit of weak flow on the volume fraction, at local scale and global scale reveal some light on the effect of initial configuration on the stable structure. Such limit aggregate at weak flow condition is typical, and more suitable to represent the restructuring of aggregate than the initial one. It is possible to predict the structure of the stable aggregate at a given fluid condition. Moreover, a specific relation between the connection capability and the strength of aggregate is established.

The effect of penetration of fluid flow on the restructuring of the aggregate is examined. The penetration of fluid flow on the aggregate is weekly dependent on porosity. Regarding the contribution of structure of aggregate on the restructuring, the structure of aggregate is apt to affect strength of aggregate compared to the fluid flow.