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# Lattice Boltzmann simulation of the dispersion of aggregated Brownian particles in shear flows

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せん断流れ場における微粒子凝集体の分散挙動を二相系格子ボルツマン法を応用した新しい微粒子分散系シミュレーション法を用いて調べた。粒子に作用する力としてファン・デル・ワールス粒子間引力とブラウン揺動力を考慮し、粒子に作用する流体抗力と粒子間凝集力の比,  $I$ , 粒子の直径とデバイ長の比,  $s$ , 流体抗力とブラウン揺動力の相対的な影響力を表すペクレ数,  $Pe$ , についてそれらのパラメータの凝集体の分散挙動への影響を調べた。

## 1 Introduction

The dispersion of small particles, especially nano-size particles, in a liquid is a key technology for making new functional materials. Small particles are easy to be aggregated by an attraction force between the particles. Thus it is difficult to disperse a large number of particles uniformly in a liquid. In addition to the attraction force the Brownian force comes to be important for nano-size particles. The characteristics of the aggregated Brownian particles in fluid flow have been unclear. In the present paper, we investigate numerically the dispersion of the aggregated Brownian particles under shear flows with using the extension to the case of Brownian particles and large number of particles of the method proposed by Inamuro and Ii [1].

## 2 Numerical Method

From a numerical point of view, this subject is a moving boundary problem and so there are some difficulties in dealing with many moving particles in a liquid. Some numerical methods for colloidal dispersion that can overcome the difficulties have been proposed recently. (e.g. [2], [3]) In our method, the solid particle is modeled by a droplet with strong interfacial tension and large viscosity, and the Lattice Boltzmann method (LBM) for multicomponent immiscible fluids is applied. In the LBM, it does not track interfaces, but can maintain sharp interfaces without any artificial treatments. Also, the LBM is accurate for the mass conservation of each component fluid. In the simulation colored droplets are introduced to avoid merging of droplets. In addition, to reduce the number of colors, a color exchanging algorithm is used; that is, a same color is allocated for particles in far distances, and, when the same colored particles get close together in the flow, the color of one is changed to the different color before their collision.

## 3 Result and Discussion

Aggregated particles with the diameter  $D$  are in a liquid inside a rectangular domain, and at  $t=0$  the top and bottom walls begin to move in the  $x$ -direction with the velocity  $u_w$  and  $-u_w$ , respectively (see Fig. 1). The periodic boundary condition is used on the other sides of the domain.

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In order to classify calculated results, we introduce following nondimensional parameters; the ratio of the hydrodynamic drag force to cohesive force,  $I = (\dot{\gamma}D^2/2)/(Ah/D)$ , the ratio of the Debye length to diameter of particle,  $s$ , and the Péclet number,  $Pe = \dot{\gamma}D^2/C_d$ , which measures the relative importance of shear and Brownian forces, where  $\eta$  is the viscosity of solvent,  $Ah$  is the Hamaker constant,  $\dot{\gamma} = 2u_w/L_z$ , and  $C_d$  is the diffusion coefficient of a single sphere at infinite dilution.

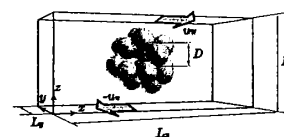


Fig. 1: Computational domain

Fig. 2 shows a comparison of deformation between aggregate of Brownian particles and that of non-Brownian particles. It is seen that the Brownian particle-cluster deforms slower than that of non-Brownian particles under shear flows. This feature is seen also for other parameter sets. The Brownian force seems to control the dispersion of aggregated particles. Fig. 3 shows the standard deviations  $\sigma$  against the parameter  $I'$ , which is defined as  $I' = s^2I$ , for the case of aggregation with 6 and 18 particles. It is found that in spite of the number of particles and the value of  $s$  the aggregates are dispersed when  $I'$  is over 0.01.

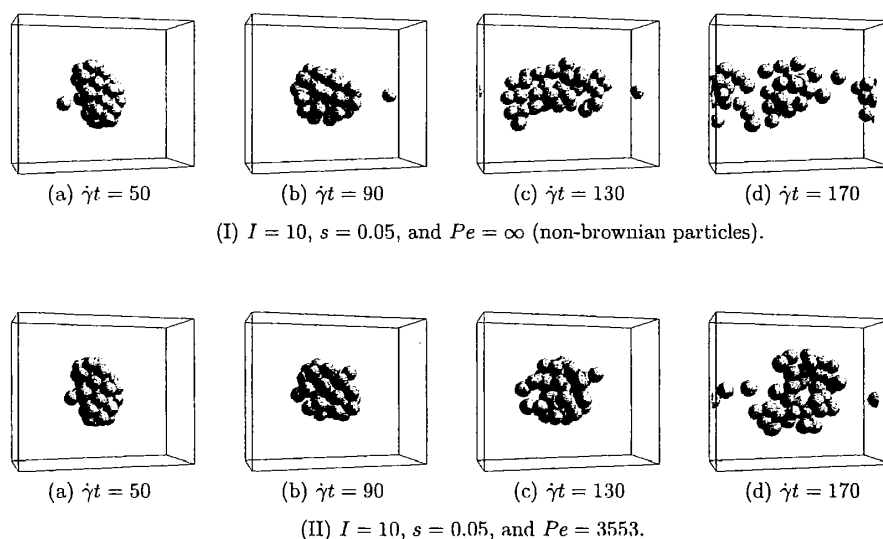


Fig. 2: Deformation of aggregate with 36 particles for  $I = 10$ ,  $s = 0.05$ , and  $Pe = \infty$  (i.e. non-Brownian particles) for the upper and  $Pe = 3553$  for the lower.

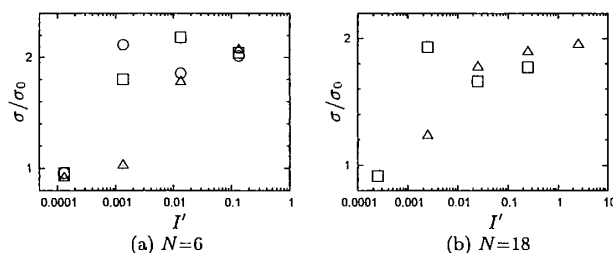


Fig. 3: Standard deviation  $\sigma$  versus  $I'$ . (a) for 6 particles at  $\dot{\gamma}t = 120$ . (b) for 18 particles at  $\dot{\gamma}t = 200$ .  $\square$ ,  $\circ$ , and  $\triangle$  indicates the result for  $s = 0.005$ ,  $0.01$ , and  $0.05$ , respectively.

## References

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