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Numerical simulation of the dispersion of aggregated Brownian particles under shear flows

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ABSTRACT

The deformation and breakup processes of a particle-cluster aggregate under shear flows are numerically investigated by the two-phase lattice Boltzmann method. The van der Waals attraction is considered to be the force between particles. Simulations are performed for various fluid forces acting on particles and various inter-particle forces. It is found that the ratio of the fluid force to the maximum inter-particle force, Y, is a key factor in dispersion, and the aggregate of non-Brownian particles is dispersed when Y is over 0.001. The Péclet number, which is the ratio of the diffusion rate due to shear flow to that due to the Brownian motion, is also considered. By comparing the calculated result of the dispersion of Brownian particles with that of non-Brownian particles, it is found that the Brownian motion impedes dispersion and the effect of the Brownian motion is remarkable when the Péclet number is under 10^5.

1. Introduction

The dispersion of micro- and nanoparticles in a liquid is important for making new functional materials such as ceramics, polymers, and electronic products because the characteristics of materials can be controlled by dispersing small particles in a solvent in their production process. However, small particles are easy to be aggregated by an attraction force between the particles, so it is difficult to disperse a large number of particles uniformly in a liquid. Therefore, to develop new functional materials, it is important to investigate particle dispersion in liquids.

The breakup mechanism of aggregated particles has been studied both experimentally and theoretically [1–5]. Because the dispersion dynamics of particles is very complicated, it is difficult to investigate the breakup mechanism of aggregated particles only through experimental and theoretical approaches, so several numerical methods have been proposed. However, in general, there are difficulties in treating a moving solid–liquid boundary even in the numerical simulations of particulate flows.

Bossis and Brady [6] proposed the Stokesian dynamics, in which a solvent fluid is not treated explicitly, but the hydrodynamic interaction between particles is treated as a resistance of the solvent fluid expressed by relative velocity vectors of the particles. Harada et al. [7] investigated the dispersion of particles by the Stokesian dynamics. However, the Stokesian dynamics remains difficult for applications with complex boundaries. Immersed boundary approaches, in which a moving boundary condition is satisfied through external forces in the Navier–Stokes equation, have been proposed [8–10]. Feng and Michaelides [11], and Melchionna [12] also proposed an immersed boundary approach combined with the lattice Boltzmann method to solve a fluid–particle interaction problem. These models using the immersed boundary method are effective approaches for moving boundary problems, but the immersed boundary method might cause numerical errors while evaluating the hydrodynamic force and torque acting on particles in various situations. Tanaka and Araki [13] proposed the fluid particle dynamics method, in which a particle is treated as a fluid with large viscosity. Although this method can eliminate the difficulty originating from the solid-liquid boundary condition, it is difficult to retain the spherical shape for a long time. Ladd [14] proposed a simulation model for moving particles using the lattice Boltzmann method in which the hydrodynamic force exerted on a particle is calculated on the basis of momentum exchange.

Recently, the two-phase lattice Boltzmann method with the same density [15] has been applied to the simulations of the dispersion of aggregated particles under shear flows by the authors [16]. In this method, the particle is modeled by a hard droplet with large viscosity and strong surface tension, and consequently, we do not need to explicitly track the moving solid–liquid boundary. Strong surface tension is applied to maintain a spherical droplet without any other artificial treatments. Some models of the lattice

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Boltzmann method that involve droplets and tunable surface tension are also available [17–20]. Here the free energy functional scheme proposed by Swift et al. [17] is used to apply strong surface tension. The advantage of the two-phase lattice Boltzmann method is its simplicity in treating the solid-liquid boundary. Zaleski et al. [21], e.g., proposed the volume-of-fluid method, which involves droplets and tunable surface tension. However, the evaluation of the boundary gradient is complex. In the two-phase lattice Boltzmann method, the boundary surface is autonomously determined to minimize the free energy of the system. In addition, a colored order parameter is assigned to each droplet for preventing the droplets from merging into bigger droplets.

In this study, we improve the above-mentioned method to treat the Brownian motion of nanoparticles and simulate a large number of particles with a smaller number of colored order parameters. Next, we use the improved method to investigate the behavior of particles under shear flows for various conditions. In general, particles diffuse by the Brownian motion in fluid, so, the Brownian motion may promote dispersion. However, it is also known that particles, which are initially separated, aggregate by the Brownian motion (see e.g., Ref. [16]). Therefore, the effect of the Brownian motion on the dispersion of initially aggregated particles is not yet clear. To classify the calculated results, we introduce two important dimensionless parameters: the ratio of the fluid force to the maximum inter-particle force and the Péclet number, which is the ratio of the diffusion rate due to shear flow to that due to the Brownian motion.

The paper is organized as follows: In Section 2, we explain the numerical method. Simulation results are presented in Section 3, in which we investigate the dispersion of the aggregations of 36 and six particles. We conclude the study in Section 4.

2. Numerical method

2.1. Two-phase lattice Boltzmann method for immiscible fluids with the same density

Non-dimensional variables are used as in Ref. [22]. The lattice kinetic scheme (LKS) [23], which is an extension method of the lattice Boltzmann methods, is used to formulate the method. In the LKS, macroscopic variables are calculated without particle velocity distribution functions, and thus the scheme can save computer memory, since there is no need to store the particle velocity distribution functions. In addition, in order to represent many hard droplets, which cannot merge into bigger droplets, we introduce colored order parameters to make different colored droplets. Differently colored droplets do not merge if they collide because the boundary surface of each colored droplet is independently and autonomously determined. Note that the color is physically meaningless and is used only for distinguishing each droplet from the others. In the present study, the Stokes flow is assumed because the diameter of a particle is very small (e.g., 1 μm).

The 15-velocity model with particle velocities $\boldsymbol{c}_i (i = 1,2,\ldots,15)$ is used in this study. The velocity vectors of this model are given by

$$[\boldsymbol{c}_1,\boldsymbol{c}_2,\boldsymbol{c}_3,\boldsymbol{c}_4,\boldsymbol{c}_5,\boldsymbol{c}_6,\boldsymbol{c}_7,\boldsymbol{c}_8,\boldsymbol{c}_9,\boldsymbol{c}_{10},\boldsymbol{c}_{11},\boldsymbol{c}_{12},\boldsymbol{c}_{13},\boldsymbol{c}_{14},\boldsymbol{c}_{15}] = \begin{bmatrix} 0 & 1 & 0 & 0 & -1 & 0 & 0 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 \\ 0 & 0 & 1 & 0 & 0 & -1 & 0 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 1 & 0 & 0 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 \end{bmatrix}. \quad (1)$$

The physical space is divided into a cubic lattice, and the colored order parameter $\phi_l(\boldsymbol{x},t)$ ($l = 1,2,\ldots,N$), where N is the number of colors, the pressure $p(\boldsymbol{x},t)$ and the velocity $\boldsymbol{u}(\boldsymbol{x},t)$ of whole fluid at the lattice point $\boldsymbol{x}$ and at time t are computed as follows:

$$\phi_l(\boldsymbol{x}, t+\Delta t) = \sum_{i=1}^{15} f_{li}^{\mathrm{eq}}(\boldsymbol{x} - \boldsymbol{c}_i\Delta x, t), \quad (2)$$

$$p(\boldsymbol{x}, t+\Delta t) = \frac{1}{3}\sum_{i=1}^{15} g_i^{\mathrm{eq}}(\boldsymbol{x} - \boldsymbol{c}_i\Delta x, t), \quad (3)$$

$$\boldsymbol{u}(\boldsymbol{x}, t+\Delta t) = \sum_{i=1}^{15} \boldsymbol{c}_i g_i^{\mathrm{eq}}(\boldsymbol{x} - \boldsymbol{c}_i\Delta x, t). \quad (4)$$

where f_{li}^{eq} and g_i^{eq} are equilibrium distribution functions, Δx is a spacing of the cubic lattice, and Δt is a time step during which the particles travel the lattice spacing.

The equilibrium distribution functions in Eqs. (2)–(4) are given by

$$f_{li}^{\mathrm{eq}} = H_i\phi_l + F_i\left[p_0(\phi_l) - \kappa_f\phi_l\nabla^2\phi_l - \frac{\kappa_f}{6}|\nabla\phi_l|^2\right] + 3E_i\phi_l c_{i\alpha}u_\alpha + E_i\kappa_f G_{\alpha\beta}(\phi_l)c_{i\alpha}c_{i\beta}, \quad (5)$$

$$g_i^{\mathrm{eq}} = E_i\left[3p + 3c_{i\alpha}u_\alpha + A\Delta x\left(\frac{\partial u_\beta}{\partial x_\alpha} + \frac{\partial u_\alpha}{\partial x_\beta}\right)c_{i\alpha}c_{i\beta}\right] + E_i\kappa_g G_{\alpha\beta}(\phi_l)c_{i\alpha}c_{i\beta} + 3E_i c_{i\alpha}\Delta x\sum_{l=1}^{N} F_{l\alpha}\Phi_l, \quad (6)$$

where

$$E_1 = 2/9, \quad E_2 = E_3 = E_4 = \cdots = E_7 = 1/9,$$
$$E_8 = E_9 = E_{10} = \cdots = E_{15} = 1/72,$$
$$H_1 = 1, \quad H_2 = H_3 = H_4 = \cdots = H_{15} = 0,$$
$$F_1 = -7/3, \quad F_i = 3E_i (i = 2,3,4,\ldots,15), \quad (7)$$

and

$$G_{\alpha\beta}(\phi) = \frac{9}{2}\frac{\partial\phi}{\partial x_\alpha}\frac{\partial\phi}{\partial x_\beta} - \frac{3}{2}\frac{\partial\phi}{\partial x_\gamma}\frac{\partial\phi}{\partial x_\gamma}\delta_{\alpha\beta}, \quad (8)$$

with $\alpha, \beta, \gamma = x, y, z$ (subscripts α, β, and γ represent Cartesian coordinates, and the summation convention is used). In the above equations, $\delta_{\alpha\beta}$ is the Kronecker delta, κ_f is a constant parameter determining the width of the interface, κ_g is a constant parameter determining the strength of the surface tension, and A is a constant parameter related to fluid viscosity. In Eq. (4), $p_0(\phi)$ is given by

$$p_0(\phi) = \phi T_\phi\frac{1}{1-b\phi} - a\phi^2, \quad (9)$$

where a, b, and T_ϕ are free parameters determining the maximum and minimum values of the order parameter, $\phi_{\max}$ and $\phi_{\min}$. It is noted that f_{li}^{eq} is the same as that for the model of Swift et al. [17], except that f_{li}^{eq} in Eq. (5) has no second terms of u_α because we assume the Stokes flow. The last term of Eq. (6) is the force $\boldsymbol{F}_l$ acting on the lth particle per unit mass:

$$\boldsymbol{F}_l = \sum_{m=1}^{N}\boldsymbol{F}_{\mathrm{v}lm} + \boldsymbol{F}_{\mathrm{Br}l}, \quad (10)$$

where $\boldsymbol{F}_{\mathrm{v}lm}$ is the attractive force per unit mass from the mth particle to the lth particle, and $\boldsymbol{F}_{\mathrm{Br}l}$ is the Brownian force per unit mass acting on the lth particle. The detailed formulations of forces are given in the following subsections. In addition, Φ_l in Eq. (6) represents the region of a droplet; i.e., it is unity inside the droplet and zero outside the droplet:

$$\Phi_l = \begin{cases} 1, & \phi_l \geqslant \phi_{\mathrm{B}}, \\ 0, & \phi_l < \phi_{\mathrm{B}}. \end{cases} \quad (11)$$

ϕ_{B} is the threshold value of the boundary and is defined as follows:

$$\phi_{\mathrm{B}} = \frac{\zeta\phi_{\min} + \phi_{\max}}{\zeta + 1}, \quad (12)$$

where ζ is a weight parameter and is described in detail in Appendix A.