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Simulation of interaction between a freely moving solid particle and a freely moving liquid droplet by lattice Boltzmann method

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ABSTRACT

Solid particles and liquid droplets widely coexist in many industrial processes. Particle-droplet interactions critically influence the dynamics of those processes. In this study, the interactions between a freely moving solid particle and a freely moving liquid droplet are numerically investigated using the lattice Boltzmann method. Until now the open literature on such topic is quite sparse. Through the present numerical investigation, two regimes to classify the interactions between a freely moving solid particle and a freely moving liquid droplet are proposed. In addition, it is found that the particle-to-droplet size ratio and particle's wettability play critical roles in such interactions.

1. Introduction

Liquid–gas–particle (LGP) systems widely exist in many industrial applications such as electronics fabrication by ink-jet printing [1] and emulsion stabilization in food [2], cosmetics [3], and petroleum industries [4,5]. In LGP systems, the interactions between droplets and particles critically influence the performance of the systems. Up to date, the particle-particle interactions have been investigated extensively [6–10]. A so-called DKT (drafting, kissing, and tumbling) process may happen during interaction between two solid particles. For collisions between two droplets, many studies [11–17] observed four types of collision regimes: bouncing, coalescence, stretching and reflexive, based on the Weber number (We) and impact parameter (b). Compared with its particle-particle and droplet-droplet counterparts, the open studies on particle-droplet interactions are relatively sparse. Shen [18] analyzed the effects of the droplet's velocity, size ratio of the droplet to solid, and temperature difference on liquid attachment during droplet-particle collisions. The authors found that the percentage of liquid attachment decreases against increasing droplet impact velocity. In addition, the authors concluded that a center-to-center collision would result in more liquid attachment than an off-center collision. Mitra et al. [19] investigated the collision behavior of a small solid particle against a large stationary droplet. They analyzed the processes of the solid particle penetrating through the droplet and claimed that the capillary force dominated the whole process. Gac et al. [20,21] investigated the influences of some dimensionless parameters, such as the Weber number, capillary number and droplet-to-particle diameter ratio, on the kinetics of central collision between a droplet and a particle. The authors observed three types of collision behavior: coalescence, ripping and coating, and skirt scattering. The authors also found that the behavior of central collision were nearly insensitive to the particle's shape. Hardalupas et al. [22] investigated the dynamics of small droplets impacting against a large solid surface. Their results showed that an impinging droplet could form a crown, which was influenced by surface roughness, droplet kinematics and liquid properties. Bakshi et al. [23] conducted experiments to investigate the effects of droplet Reynolds number and particle-to-droplet size ratio on the behavior of a liquid film on a solid surface. Three transitional phases of the film kinetics, namely the initial drop deformation phase, inertia dominated phase, and viscosity dominated phase, were observed. Fakhari and Bolster [24] conducted a simulation for a droplet's impingement on a hydrophilic or superhydrophobic cylinder under gravity. Their results indicated that a droplet tended to adhere to the surface of a hydrophilic cylinder while it tended to break up and detach from the surface of a hydrophobic cylinder. Malgarinos et al. [25] simulated the impact

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processes of a liquid droplet against a spherical stationary solid particle. Two different regimes: the partial/full rebound and coating regime were identified. Malgarinos et al. [26,27] investigated the collisions between heavy gasoil droplets and solid catalytic particles. In their studies, phase-change phenomena and catalytic cracking surface reactions were taken into account.

In the all above-mentioned studies, the investigated solid particles or liquid droplets are stationary, rather than freely moving. For the scenarios where both a particle and a droplet can freely move, Dubrovsky et al. [28] carried out a pioneering experimental study on particle-droplet collisions. For the cases where the droplet-to-particle size ratio was greater than 1, they observed four collision modes: particle capture, "shooting through" with satellite droplet formation, "shooting through" with gas bubble formation and droplet destruction. Then, Deen et al. [29] simulated collisions of a falling particle against a rising bubble by a front tracking approach combined with an immersed boundary (IB) scheme. They studied the effect of particle's density on the interaction between the particle and the bubble. Higher particle's density led to more significant deformation of the bubble and increasing the possibility of the particle penetrating through the bubble. In their work, only head-on collisions were considered. Sasic et al. [30] numerically studied the interaction between settling particles and rising microbubbles. They observed that the particles would attach to the bubbles when the initial horizontal distance between their centers was small enough, while the particles would pass through the bubbles if such initial distance was large. Kan et al. [31] simulated the processes of particle-particle combination by a droplet. The authors discussed the effect of particle's wettability on the critical velocity for particle-particle combination. They concluded that such critical velocity varied non-monotonically with the particle's wettability. They also investigated the effect of droplet size on the adhesiveness of two colliding particles [32]. It was found that against the increasing of droplet's diameter, the adhesiveness of particles became weak. Recently, Pawar et al. [33] experimentally investigated particle-droplet collisions at low capillary numbers. The collision behavior was classified into two regimes: agglomeration (merging) and stretching separation (breaking), based on the Weber number and impact parameter. In addition, they proposed a map based on the droplet-to-particle size ratio to illustrate the regimes.

Through the above literature survey, it is clear that the open literature on interactions between a freely moving droplet and a freely moving particle is extremely sparse. In addition, the in-depth knowledge about the effect of particle's wetting property on particle-droplet collisions is still absent. To bridge the gap, in this study, the interactions between a freely moving particle and a freely moving droplet are investigated numerically. Moreover, the effects of particle's wettability on collision behavior are also discussed.

2. Numerical method

It is difficult to conduct experiments to study interactions between a freely moving solid particle and a freely moving droplet, so numerical methods are chosen for the present research. Until now the lattice Boltzmann method (LBM) has matured to model particle dynamics [6–10] and multi-phase multi-component flow [34–39]. Consequently, in this work the LBM-based Shan-Chen multi-phase multi-component (MCMP) model [34] is adopted for simulating liquid droplets and the LBM-based particle dynamics modelling approach [40] is employed for simulating particle's motion.

2.1. Multiphase flow

In the MCMP model, the pseudo fluid particle distribution function (PDF) for each fluid component satisfies [34]:

$$f_i^\sigma(\mathbf{x}+\mathbf{e}_i\Delta t, t+\Delta t) = f_i^\sigma(\mathbf{x},t) - \frac{1}{\tau_\sigma}(f_i^\sigma(\mathbf{x},t) - f_i^{\sigma,eq}(\mathbf{x},t)) \tag{1}$$

where $f_i^\sigma(\mathbf{x},t)$ is the PDF for the σth fluid component and τ_σ is its relaxation time, which is determined by the kinematic viscosity as $\upsilon_\sigma = c_s^2(\tau_\sigma - 0.5\Delta t)$. $f_i^{\sigma,eq}(\mathbf{x},t)$ is the equilibrium distribution function and can be expressed as

$$f_i^{\sigma,eq}(\mathbf{x},t) = \omega_i\rho_\sigma\left[1 + \frac{\mathbf{e}_i\cdot\mathbf{u}_\sigma^{eq}}{c_s^2} + \frac{(\mathbf{e}_i\cdot\mathbf{u}_\sigma^{eq})^2}{2c_s^4} - \frac{\mathbf{u}_\sigma^{eq2}}{2c_s^2}\right] \tag{2}$$

where $\omega_0 = 4/9$, $\omega_{1\text{-}4} = 1/9$ and $\omega_{5\text{-}8} = 1/36$, and $\mathbf{e}_i$ is the discrete velocity. For the D2Q9 model $\mathbf{e}_i$ is defined as

$$\mathbf{e}_i = \begin{cases} (0,0) & i = 0 \\ c(\cos[(i-1)\pi/2], \sin[(i-1)\pi/2]) & i = 1,2,3,4 \\ \sqrt{2}c(\cos[(2i-1)\pi/4], \sin[(2i-1)\pi/4]) & i = 5,6,7,8 \end{cases} \tag{3}$$

In this paper $c = \Delta x = \Delta t = 1$. The macroscopic density ρ_σ and velocity $\mathbf{u}_\sigma$ for the σth fluid component are obtained by

$$\rho_\sigma = \sum_i f_i^\sigma, \mathbf{u}_\sigma = \frac{1}{\rho_\sigma}\sum_i \mathbf{e}_i f_i^\sigma \tag{4}$$

The equilibrium velocity $\mathbf{u}_\sigma^{eq}$ is calculated by

$$\mathbf{u}_\sigma^{eq} = \mathbf{u}^c + \frac{\tau_\sigma \mathbf{F}_\sigma}{\rho_\sigma} \tag{5}$$

where $\mathbf{u}^c$ is the composite macroscopic velocity and given by

$$\mathbf{u}^c = \frac{\sum_\sigma \frac{1}{\tau_\sigma}\sum_i f_i^\sigma \mathbf{e}_i}{\sum_\sigma \frac{\rho_\sigma}{\tau_\sigma}} \tag{6}$$

The pressure P is obtained by

$$P = (\rho_\sigma + \rho_{\bar\sigma})c_s^2 + 3Gc^2\rho_\sigma\rho_{\bar\sigma} \tag{7}$$

The inter-particle force on the σth component is defined as [36]

$$F_{\text{int},\sigma}(\mathbf{x},\mathrm{t}) = -G\rho_\sigma(\mathbf{x},\mathrm{t})\sum_i \omega_i\rho_{\bar\sigma}(\mathbf{x}+\mathbf{e}_i\Delta\mathrm{t},\mathrm{t})\mathbf{e}_i \tag{8}$$

where the σ and $\bar\sigma$ indicate two different fluid components and G is a parameter that controls the interaction strength of inter-particle force.Solid surface forces are incorporated into the MCMP model through

$$F_{\text{ads},\sigma}(\mathbf{x},\mathrm{t}) = -G_{\text{ads},\sigma}\rho_\sigma(\mathbf{x},\mathrm{t})\sum_i \omega_i s(\mathbf{x}+\mathbf{e}_i\Delta\mathrm{t},\mathrm{t})\mathbf{e}_i \tag{9}$$

where s is an indicator function, which equals to 1 or 0 for a solid or fluid node, respectively. The parameter G_{ads} controls the interaction strength between fluid and solid nodes.

To reduce the spurious velocity currents, we adopt the improvement scheme of sufficient isotropy (up to 8 order) to calculate the gradient of the density [35] and the explicit forcing (EF) scheme to discrete the inter-particle force [37,39].

2.2. Particle treatment

In this work we adopt the half-way bounce back scheme for particle boundary treatment as it can guarantee mass conservation during simulation. Boundary nodes are located at the midway between a fluid node and a solid node. The normal streaming step happens when pseudo fluid particles stream from a fluid node to a neighboring fluid node. If the adjacent node of a fluid node is solid, the half-way bounce-back scheme acts as

$$f_{\bar i}(\mathbf{x}, t+1) = f_i^+ - 6\rho_w\omega_i(\mathbf{u}_b\cdot\mathbf{e}_i) \tag{10}$$

where $\bar i$ indicates the direction opposite to i, $\mathbf{u}_b$ is the velocity of the boundary node and ρ_w is set to be the density of external fluid node.