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A three-dimensional pseudo-potential-based lattice Boltzmann model for multiphase flows with large density ratio and variable surface tension

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ABSTRACT

In this paper, we present a three-dimensional pseudo-potential-based lattice Boltzmann (LB) model with an improved forcing scheme for multiphase flows. The Chapman–Enskog multiscale analysis shows that the proposed forcing scheme allows the lattice Boltzmann equation to recover the three-dimensional hydrodynamical equations with additional terms that correspond to the mechanical stability condition and surface tension. Validations of the present LB model with Maxwell construction, Laplace's law and oscillation dynamics demonstrate that the model enables the density ratio to be as large as 700 in static and quasi-static cases while maintaining variable surface tension. Finally, the application of the model to simulation of the droplet motion in a microchannel shows that the model allows the analysis of important effects, including droplet surface tension, channel surface wettability, and channel surface roughness.

1. Introduction

A great deal of numerical studies on multiphase flows have been done during the past decades, and they have attracted much attention recently because of their wide applications in microfluidics devices (Cheng et al., 2014). Traditionally, multiphase flows are simulated by solving the macroscopic Navier–Stokes equations coupled with various approaches to track the interface among different phases. Generally, these approaches are classified into two categories: one is the interface-tracking approach, i.e., using Lagrangian approach to explicitly represent the interface, such as the front tracking method (Unverdi and Tryggvason, 1992), while the other is the interface-capturing approach, i.e., using Eulerian approach to implicitly represent the interface by a scalar function, such as the volume of fluid method (Hirt and Nichols, 1981), the level set method (Sethian and Smereka, 2003), and the phase field method (Badalassi et al., 2003). However, simulation of multiphase flows based on the Navier–Stokes equations remains a challenging issue as it is difficult to track complex phase interfaces that physically result from microscopic interactions between molecules (Sbragaglia et al., 2006).

Alternatively, due to its kinetic nature, the lattice Boltzmann (LB) method has proved to be a promising tool for simulating fluid systems involving interfacial dynamics (such as multiphase flows) and complex boundaries (such as porous media) (Chen and Doolen, 1998). Existing LB models for multiphase flows can be generally classified into four categories: the color-gradient model (Gunstensen et al., 1991; Grunau et al., 1993), the pseudo-potential model (Shan and Chen, 1993; Shan and Chen, 1994), the free-energy model (Swift et al., 1995; Swift et al., 1996), and the kinetic-theory-based model (He et al., 1998; He and Doolen, 2002). Among those models, the pseudo-potential model, which is also called Shan–Chen model, has received much attention, primarily because interfaces can naturally arise, deform, and migrate, thereby improving the computational efficiency (Chen et al., 2014; Succi, 2015). Specifically, the fluid interactions are described by an artificial inter-particle potential and the phase separation is naturally achieved by imposing a short-range attraction among different phases. However, there are two issues associated with the pseudo-potential model proposed by Shan and Chen (1993, 1994). One is that this model is applicable to low-density-ratio interfacial problems only (Yuan and Schaefer, 2006), while the other is that in this model surface tension cannot be varied independently of the density ratio (Sbragaglia et al., 2007). Over the past years, efforts have been made to address these issues (Yuan and Schaefer, 2006; Sbragaglia et al., 2007; Shan, 2006; Huang et al., 2011; Li et al., 2012; Li et al., 2013; Li and Luo, 2013). For

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instance, one of previous efforts is to incorporate the fluid interaction force into the pseudo-potential model via improving the forcing scheme (Huang et al., 2011; Li et al., 2012; Li et al., 2013; Li and Luo, 2013). Li et al. (2013) proposed a forcing scheme for a two-dimensional (2D) multiple-relaxation-time (MRT) pseudo-potential LB model. This forcing scheme can adjust the mechanical stability condition so that multiphase flows with a large density ratio can be simulated. In addition, Li and Luo (2013) also proposed to adjust the surface tension in the 2D MRT pseudo-potential LB model by incorporating a source term of the LB equation, which is based on the derivation of discrete form pressure tensor. As a practical numerical tool for simulating engineering problems, however, it is desirable to extend 2D models to three-dimensional (3D) models to truly reflect the real-world multiphase flow behaviors. However, as the underlying lattice structure for 2D and 3D models are different, there are significant differences in the development and implementation of 3D MRT models (Premnath and Abraham, 2007).

In this work, we extend the 2D forcing scheme proposed by Li et al. (2013) and Li and Luo (2013) to 3D MRT pseudo-potential LB model for single-component multiphase flows with a large density ratio and variable surface tension. The rest of the paper is organized as follows: In Section 2, we present the pseudo-potential LB model and give the new forcing scheme, followed by the Chapman–Enskog analysis to derive macroscopic equations. In Section 3, the present multiphase LB model is evaluated by verifying Maxwell construction, Laplace's law, spurious velocities, spatial accuracy, oscillation dynamics and contact angle, respectively. After that, numerical simulations are carried out to study liquid droplets moving in a 3D microchannel, including the effects of droplet surface tension, channel surface wettability, and channel surface roughness.

2. Numerical method

2.1. Two-phase lattice Boltzmann method

2.1.1. The multiple-relaxation-time LB model

The evolution equation of LB model can be written as

$$f_i(\mathbf{x}+\mathbf{e}_i\delta_t, t+\delta_t) - f_i(\mathbf{x},t) = \Omega_i + \delta_t F_i' \tag{1}$$

where f_i is the density distribution function, t is the time, $\mathbf{x}$ is particle position, $\mathbf{e}_i$ is the discrete velocity along the ith direction, δ_t is the time step, F_i' is the forcing term in velocity space, Ω_i is the collision operator which can be expressed by either Bhatnagar–Gross–Krook (BGK) collision operator (Qian et al., 1992) or multiple-relaxation-time (MRT) collision operator (Lallemand and Luo, 2000; d'Humières, 2002). In this work, we adopt MRT collision operator for its superior numerical stability over BGK collision operator in simulating both single and multiphase flow (Premnath and Abraham, 2007; Lallemand and Luo, 2000; d'Humières, 2002; Chai and Zhao, 2012). The MRT collision operator Ω_i is defined as

$$\Omega_i = -(\mathbf{M}^{-1}\mathbf{S}\mathbf{M})_{ij}\left[f_j(\mathbf{x},t) - f_j^{(\mathrm{eq})}(\mathbf{x},t)\right] \tag{2}$$

For the D3Q15 lattice model, $\mathbf{e}_i$ can be given as

$$[\mathbf{e}_0,\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3,\mathbf{e}_4,\mathbf{e}_5,\mathbf{e}_6,\mathbf{e}_7,\mathbf{e}_8,\mathbf{e}_9,\mathbf{e}_{10},\mathbf{e}_{11},\mathbf{e}_{12},\mathbf{e}_{13},\mathbf{e}_{14}] = c\begin{bmatrix} 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \end{bmatrix} \tag{3}$$

where $c = \delta_x/\delta_t$ is lattice constant. $\mathbf{M}$ is orthogonal transformation matrix, given by d'Humières (2002)

$$\mathbf{M} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -2 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 16 & -4 & -4 & -4 & -4 & -4 & -4 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 0 & -4 & 4 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & 0 & -4 & 4 & 0 & 0 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & -4 & 4 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 0 & 2 & 2 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{bmatrix} \tag{4}$$

and $\mathbf{S}$ is a relaxation matrix. To keep the relaxation matrix $\mathbf{S}$ consistent with the moment, we write it as $\mathbf{S} = \mathrm{diag}(s_\rho, s_e, s_\epsilon, s_j, s_q, s_j, s_q, s_j, s_q, s_v, s_v, s_v, s_v, s_v, s_{xyz})$.

The density distribution function f_i and its equilibrium distribution $f_i^{(\mathrm{eq})}$ can be projected onto moment space via $\mathbf{m} = \mathbf{M}\mathbf{f}$ and $\mathbf{m}^{(\mathrm{eq})} = \mathbf{M}\mathbf{f}^{(\mathrm{eq})}$, respectively. Thus, the evolution equation of density distribution function can be rewritten as

$$\mathbf{m}^* = \mathbf{m} - \mathbf{S}(\mathbf{m} - \mathbf{m}^{(\mathrm{eq})}) + \delta_t\left(\mathbf{I} - \frac{\mathbf{S}}{2}\right)\mathbf{M}\tilde{\mathbf{F}} \tag{5}$$

where $\mathbf{I}$ is the unit tensor and $\mathbf{M}\tilde{\mathbf{F}}$ is the forcing term in the moment space with $(\mathbf{I} - 0.5\mathbf{S})\mathbf{M}\tilde{\mathbf{F}} = \mathbf{M}\mathbf{F}'$, the equilibrium $\mathbf{m}^{(\mathrm{eq})}$ is given by

$$\mathbf{m}^{(\mathrm{eq})} = \rho\Big(1, -1 + |\mathbf{u}|^2, 1 - 5|\mathbf{u}|^2, u_x, -\frac{7}{3}u_x, u_y, -\frac{7}{3}u_y, u_z, -\frac{7}{3}u_z, 2u_x^2 - u_y^2 - u_z^2, u_y^2 - u_z^2, u_xu_y, u_yu_z, u_xu_z, 0\Big)^T \tag{6}$$

where u_x, u_y and u_z denote the fluid velocity components in the (x,y,z) Cartesian coordinate system, and $|\mathbf{u}|^2 = u_x^2 + u_y^2 + u_z^2$.

The macroscopic density ρ and velocity $\mathbf{u}$ are obtained from

$$\rho = \sum_i f_i, \quad \rho\mathbf{u} = \sum_i \mathbf{e}_i f_i + \frac{\delta_t}{2}\mathbf{F} \tag{7}$$

where $\mathbf{F} = (F_x, F_y, F_z)$ is the total force acting on the system.

2.1.2. Pseudo-potential model

For single-component multiphase flows, the interaction force mimicking molecular interactions, is given by Shan (2006, 2008)

$$\mathbf{F}_{\mathrm{int}}(\mathbf{x}) = -G\psi(\mathbf{x})\sum_{i=1}^{N} w(|\mathbf{e}_i|^2)\psi(\mathbf{x}+\mathbf{e}_i)\mathbf{e}_i \tag{8}$$

where $\psi(\mathbf{x})$ is the interaction potential, G is the interaction strength, and $w(|\mathbf{e}_i|^2)$ are the weights. For the case of nearest-neighbor interactions on D3Q15 lattice, $w(1) = 1/3$, $w(3) = 1/24$ and $N = 14$.

In the pseudo-potential model, the interaction force is usually incorporated via a forcing scheme, which affects the numerical accuracy and stability of the model. In this study, we extend the forcing scheme proposed by Li et al. (2013) and Li and Luo (2013) to D3Q15 lattice. The evolution equation of density distribution function is written as

$$\mathbf{m}^* = \mathbf{m} - \mathbf{S}(\mathbf{m} - \mathbf{m}^{(\mathrm{eq})}) + \delta_t\left(\mathbf{I} - \frac{\mathbf{S}}{2}\right)\mathbf{M}\tilde{\mathbf{F}} + \mathbf{C} \tag{9}$$

where the term $\mathbf{M}\tilde{\mathbf{F}}$ and $\mathbf{C}$ are given by