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A lattice Boltzmann model for multi-component two-phase gas-liquid flow with realistic fluid properties

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ABSTRACT

Multi-component multi-phase flows are of significant interests in nature and engineering problems of different fields. Modeling the phenomena involved in multi-phase flows is challenging, attributed to the complexity in simulating phase interface dynamics and diffusion processes. Owing to its kinetic nature, lattice Boltzmann (LB) method emerges as an attractive computational approach, in dealing with complicated fluid flow problems and microstructure geometries with effectiveness of parallelized processing. However, some critical drawbacks of basic multi-phase LB models, such as the low density and kinematic viscosity ratios, thermodynamic inconsistency, and dependence of surface tension and density distribution on relaxation times, limit its application in realistic multi-component multi-phase systems. Based on the original pseudopotential model and progresses in single-component multi-phase model, a multi-component LB model was proposed to study the two-phase gas-liquid flow with realistic fluid properties. The importance of improved model is in simultaneously realizing the realistic fluid flow characteristics for multi-component two-phase system, including high density and viscosity ratios, good thermodynamic consistency, independently tunable surface tension and appropriate two-phase boundaries. The proposed LB model is validated with Laplace law and visualization experiment results, and the effects of surface tension, gas flow velocity and wall wettability on dynamic behaviors of fluid flow are investigated.

1. Introduction

Multi-component multi-phase (MCMP) flows are ubiquitous in the natural environment and industrial areas, which are generally classified as gas-liquid, gas-solid and liquid-solid flows according to the state of different components or phases [1,2]. This paper attempts to present a comprehensive multi-component model focusing on the realistic two-phase gas-liquid flows, and study the flow phenomena with the example of liquid droplet flow in gas channel.

Dynamic behaviors of two-phase flow are complicated, since it involves the physical processes of component diffusion and phase transition, as well as the dynamical variations of interface between liquid and gas phases. The fluid flow is affected by multi acting forces and structural properties, and the complexity of such system significantly increases with the inclusion of extra fluid component, such as the liquid droplet motion in presence of water vapor and air. Traditional macroscopic computational fluid dynamics (CFD) methods are difficult to simulate such complicated fluid systems, because the equation of state (EOS) around the phase interface is hard to be physically determined. Although current interface-tracking or interface-capturing techniques, such as boundary-fitted grid method [3,4], boundary element method [5,6], level set method [7,8] and volume of fluid method [9–11], are capable of describing dynamic evolutions of few large interface by costing high computational source, while the information of numerous tiny-dispersive interfaces is often missed.

Essentially, macroscopic dynamic behaviors of fluid flow are results of microscopic interactions between different components or phases. Mesoscopic methods are therefore expected to give more accurate descriptions in capturing the phase interface and modeling its dynamic variations with acceptable computational cost. Lattice Boltzmann (LB) method is a powerful technique for modeling interfacial phenomena in MCMP flows, which is based on the mesoscopic kinetic theory, and more efficient than other traditional methods, such as the competency of handling complicated solid-geometric boundaries and effortlessness of parallel computing [12]. Among different multi-phase LB models, Shan-Chen pseudopotential model is widely adopted due to its simplic-

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ity and versatility. In this model, interaction forces between different fluids or between fluid and solid are usually realized with the defined density-dependent pseudopotential. By introducing the short-range attraction into the interaction force, automatic phase separation is achieved, so phase interface is no longer needed to be bounded by the complicated explicit interface-tracking or interface-capturing techniques.

Traversed the research literatures with key word "lattice Boltzmann multi-component", no multi-component Shan-Chen LB model is found to study the droplet flow in gas channel, except one recent published work [13], which investigated the droplet coalescence phenomena with the multi-component two-phase model. Single-component LB model is universally adopted in previous modeling works, by considering the liquid water and air as two different phases [14–17]. Based on the single-component and two-phase Shan-Chen model, Han et al. [14,15] investigated the effects of wall contact angle, gas flow velocity, initial droplet distance, and different micropore combinations on liquid droplet transport behaviors, as well as the dynamic characteristic of liquid droplet motion at the corner of straight and semicircular channels. Amara and Nasrallah [16] developed a single-component and two-phase Shan-Chen model to study the effect of capillary number and wall wettability on droplet motion. Liu and Cheng [17] using the improved double distribution function thermal LB method, studied the dynamic behaviors of three-dimensional (3D) condensing droplets on the two-dimensional (2D) cold spot at a constant subcooled temperature, including their periodic formation, growth and movement. These models successively captured the details in phase interface dynamics and presented a more microscopic view of two-phase flows.

However, all of above models are based on the original pseudopotential model, which suffers from some deficiencies in modeling realistic two-phase fluid flow, such as the relatively large spurious current, low density and kinematic viscosity ratios, thermodynamic inconsistency, coupling effect between the EOS and surface tension, and dependence of surface tension and density ratio on the viscosity [18,19]. These limitations may have insignificant effect on the two-phase flow inside porous media due to the dominate role of surface tension, however, compared to the porous media with micropores, the capillary number in channel flow is usually much larger because of the increased physical size, so the effect of density and viscosity ratios cannot be ignored. Besides, in these two-phase models, a periodic boundary condition is often applied and flow is driven by a defined body force, this treatment can elimite the diverging problem, caused by large spurious velocity of phase interface when the droplet is touching such boundaries. But such a set up cannot simulate two-phase flows in channel that are driven by pressure difference or fully developed flow, with non-periodic boundaries. It is therefore important to derive appropriate boundary conditions and apply them to properly simulate two-phase flow. So the results in current publications for two-phase fluid flow in flow channel, as well as other two-phase fluid systems, are still questionable.

At the best of authors' knowledge, there is still no LB model can successfully simulate the multi-component two-phase (MCTP) fluid flow within realistic density and viscosity ratios, and appropriate capillary and Reynolds numbers. In the most recent years, considerable efforts were devoted to the improvement of original Shan-Chen model, high density and viscosity ratios between liquid and gas phases, good thermodynamic consistency and independent adjustment of surface tension have been realized in different publications [20–26], respectively, while these researches are limited to the static case or single-component multi-phase (SCMP) model. In this study, modified Shan-Chen model is comprehensively optimized to simultaneously realize these characteristics related to realistic two-phase flow, and make the model run stably in multi-component condition. The improved model is applied to study the droplet flow in flow channel to check its applicability, combined with the modified two-phase boundaries to remove the droplet from outlet with appropriate shape in realistic flow case, and different structural and operative conditions are discussed.

This paper is organized as the following parts: Section 2 roughly reviews the original Shan-Chen model and introduces the improvements aiming at original drawbacks; Section 3 validates the model with visualization experiment results and analyzes the simulation results of various conditions; and Section 4 makes a sumarization.

2. Model formulation

2.1. Physical problems

Droplet flow in flow channel is the typical two-phase gas-liquid flow and selected as calculation example to check the model's applicability. Such flow channel exists in many engineering applications, such as proton exchange membrane (PEM) fuel cells and heat exchangers. In this study, the effects of surface tension, gas flow velocity and wall contact angle are studied based on the improved MCTP LB model, to capture the droplet dynamic behaviors inside flow channel. The schematic diagram of computational domain and two-phase boundaries is shown in Fig. 1.

2.2. Original Shan-Chen model

Start from the fluid flow physics, the basic idea of LB method is to discretize the fluid and space into a series of particle and regular lattice point, and fluid particles are prescribed to collide and migrate at these lattice points based on the simple rule. Macroscopic fluid properties, such as density, velocity and temperature, are calculated by statistically averaging the specific distribution function of these particles [27,28]. In this study, only the evolution equation of density distribution function is solved, based on the assumption of isothermal flow condition and fact that convective flow is dominate in gas channel.

By considering single relaxation time Bhatnagar–Gross–Krook collision operator and a general forcing term in the LB model, the evolution equation of density distribution function can be written as:

$$f_{\sigma,\alpha}(x+\mathbf{e}_\alpha\Delta t, t+\Delta t) - f_{\sigma,\alpha}(x,t) = -\frac{1}{\tau_\sigma}\left(f_{\sigma,\alpha}(x,t) - f_{\sigma,\alpha}^{\mathrm{eq}}(x,t)\right) + \mathbf{F}_{\sigma,\alpha} \tag{2.1}$$

where $f_{\sigma,\alpha}(x,t)$ is the density distribution function, σ the component, x the spatial position, t the lattice time, τ_σ the non-dimensional relaxation time, α the velocity direction, and $\mathbf{F}_{\sigma,\alpha}$ the forcing term of σ component. For the D2Q9 lattice (Fig. 1), the discrete velocity $\mathbf{e}_\alpha$ along the α direction can be written as:

$$\mathbf{e}_\alpha = \begin{cases} 0 & \alpha = 0 \\ \left(\cos\left[\frac{(\alpha-1)\pi}{2}\right], \sin\left[\frac{(\alpha-1)\pi}{2}\right]\right) & \alpha = 1,2,3,4 \\ \sqrt{2}\left(\cos\left[\frac{(\alpha-5)\pi}{2}+\frac{\pi}{4}\right],\ \sin\left[\frac{(\alpha-5)\pi}{2}+\frac{\pi}{4}\right]\right) & \alpha = 5,6,7,8 \end{cases} \tag{2.2}$$

The equilibrium distribution function $f_{\sigma,\alpha}^{\mathrm{eq}}$ is given by:

$$f_{\sigma,\alpha}^{\mathrm{eq}} = \omega_\alpha \rho_\sigma \left[1 + \frac{\mathbf{e}_\alpha \cdot \mathbf{u}_\sigma^{\mathrm{eq}}}{c_s^2} + \frac{\mathbf{e}_\alpha \cdot \mathbf{u}_\sigma^{\mathrm{eq2}}}{2c_s^4} - \frac{\mathbf{u}_\sigma^{\mathrm{eq2}}}{2c_s^2}\right] \tag{2.3}$$

where for D2Q9 lattice, weights ω_α are given by $\omega_0 = 4/9$, $\omega_{1-4} = 1/9$ and $\omega_{5-8} = 1/36$, and sound speed $c_s = (\Delta x/\Delta t)/\sqrt{3}$, Δx and Δt are usually set as unit in non-dimensional LB modeling. Macroscopic fluid density and velocity can be obtained as: