



Hybrid lattice Boltzmann finite difference model for simulation of phase change in a ternary fluid

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ABSTRACT

In this paper, a hybrid lattice Boltzmann finite difference model based on the phase-field lattice Boltzmann and finite difference approaches is proposed to model phase-change phenomena in a ternary system. The system contains three immiscible incompressible fluids and the phase-change process happens at the interfaces of the fluids. Three distribution functions are used in the model; two of which are used to track the interfaces among three fluids and the other one is employed to recover the hydrodynamic properties (pressure and momentum). A sharp-interface energy equation is solved based on a finite difference approach and the net heat flux at the interface is considered as the driving force for the phase-change process. The proposed model is validated against available results and good agreement is found.

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1. Introduction

Phase-change phenomena occur frequently in nature and many engineering systems such as steam cycle in a steam power plant, water purification, heating and cooling systems, just to name a few. The growing presence of the phase-change phenomena (either evaporation or condensation) indicates the importance of attaining high performance thorough knowledge of the underlying physics. Although experiments can reveal some aspect of a phase-change process, it is impossible to investigate all involved parameters and their effects on the process individually. As an alternative, numerical simulations can overcome most of the limitations that experiments face. In numerical modeling of multiphase (or multi-component) fluid flows, major challenges include phase segregation, interfacial dynamics, and phase change. Generally, there are two different approaches for simulating multiphase fluid flows: interface-tracking approach (based on the Lagrangian description of the interface motion) and interface-capturing approach. Although the former enables predicting the exact location of interface, the application of this approach is limited in the high topological changes of interface. However, the latter has been demonstrated to be applicable in strong interface deformations, makes the approach to be more popular than the former. Interface capturing approach can be divided into two categories:

sharp-interface methods such as volume of fluid (VOF) [1], level set [2], and front tracking [3], and diffuse-interface methods such as phase-field [4,5] and second gradient theory [6]. In the following we present a brief overview on some binary phase-change models.

Based on the VOF method, Welch and Wilson [7] proposed a model for simulating phase-change process and employed their model for studying film boiling. However, the accurate calculation of the interface curvature is difficult in their model. Son and Dhir [8] proposed their phase-change model based on the level set method. They simulated the nucleate boiling on a horizontal surface. Because of implementing the level set method, their model suffers from lack of mass conservation. Jamet et al. [6] presented a phase-change model based on the second gradient theory. Due to thermodynamically consistent behavior of this model, the phase-change process and the topological changes of interface can be determined by solving a single set of partial differential equations (PDEs) without special treatment. It is worth mentioning that based on the VOF and level set methods, some improved variants which combine these two methods have also been proposed, e.g. the models proposed by Tomar et al. [9] and Guo et al. [10].

In the past two decades, the lattice Boltzmann method (LBM) has emerged as a promising alternative to the traditional computational fluid dynamics (CFD) based on the Navier-Stokes (NS) equations for simulating fluid flows. By incorporating the interfacial and intermolecular forces at the mesoscopic level, the LBM can readily tackle multiphase multicomponent fluid flows [11,12] which are difficult to handle by use of traditional CFD models. The LBM also

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demonstrates other advantageous over the traditional NS-based solver models such as easy of handling complex boundaries [13] and easy of parallelization [14].

So far, several phase-change lattice Boltzmann (LB) models have been proposed which can model phase-change process occurring in binary systems. Safari et al. [15] extended the phase-field LB model proposed by Lee and Liu [16] to simulate evaporation phenomenon. They modified the convection-diffusion Cahn-Hilliard (CH) equation to account for the phase-change process by introducing a source term. They utilized a diffuse-interface approach for solving the temperature field and the mass generated due to phase change are distributed on all nodes located within the interfacial region. Their model was successfully validated against the one-dimensional Stefan problem for density ratio up to 1:1000. They also simulated evaporation of a two-dimensional (2D) droplet by assuming that the droplet temperature remains constant (saturation temperature). Based on this model, several phase-change problems have been simulated [17,18]. Recently, Mohammadi-Shad and Lee [19] extended a two-phase lattice Boltzmann method to model liquid-vapor phase-change phenomenon using a sharp-interface energy solver. Unlike Safari's model [15], the proposed model in Ref. [19] distributes the generated mass on nodes around the interfaces and also there is no need to define an *ad hoc* rule for phase-field variable. The developed model was successfully validated for the Stefan and interface sucking problems. An extensive review of multiphase multicomponent LB models and phase-change LB models can be found in Ref. [20]. Most recently, Haghani et al. [21] proposed a robust ternary LB model based on Lee's binary model [16] which can tackle both partial and total spreading systems with high density ratio of 1:1000. Their model was validated against available data and good agreement was found. Based on this model, in this study, we propose a hybrid lattice Boltzmann finite difference model for simulation of phase change in a ternary system. The present model takes advantage of the sharp-interface energy solver proposed in [19]. In spite of appearance of phase-change process in ternary systems such as condensation on oil-infused rough surfaces [22,23], with no claim of completeness, to the authors' knowledge, it is the first time that a phase-change process in a ternary system is modeled numerically in the LB framework.

The rest of the paper is organized as follows. In Section 2 the derivation of the Cahn-Hilliard equations in the presence of phase change for a system consisting of three fluids is presented. Sections 3–6 present mathematical modeling for lattice Boltzmann equations (LBEs), volumetric mass flow rate, heat transfer equation, and surface tension force, respectively. Numerical validation of the model is presented in Section 7. Summary and concluding remarks are reported in Section 8.

2. Ternary Cahn-Hilliard model in the presence of phase change

In this section, a phase-field model based on the Cahn-Hilliard approach is presented for ternary fluids in the presence of phase change. To meet this goal, the continuity equation for each fluid is first presented and then the ternary Cahn-Hilliard equation proposed in Refs. [21,24] is extended to take into account the phase-change phenomenon which occurs at the interfaces. Consider a domain Ω of three incompressible, immiscible fluids. Each fluid of the mixture is distinguished by its phase-field variable (in other words, volume fraction) $\phi_i = \tilde{\rho}_i / \rho_i$, where $\tilde{\rho}_i$ and ρ_i are the local and bulk densities of fluid i , respectively, and the local average density is $\rho = \sum_{i=1}^3 \tilde{\rho}_i$. The phase-field variables are restricted by following constraint:

$$\sum_{i=1}^3 \phi_i = 1; \quad 0 \leq \phi_1, \phi_2, \phi_3 \leq 1 \quad (1)$$

The continuity equation of each fluid can be written as [15]

$$\frac{\partial \tilde{\rho}_i}{\partial t} + \nabla \cdot \mathbf{n}_i = \dot{m}_i''' \quad (2)$$

where t is the time, \mathbf{n}_i is the mass flow rate of fluid i , and \dot{m}_i''' is the volumetric source or sink of fluid i due to phase change. In the bulk region, the mass flow rate is due to convection, i.e., $\mathbf{n}_i = \tilde{\rho}_i \mathbf{u}$ where \mathbf{u} is the volume average velocity of the flow. However, in the interfacial region, another term comes into play as a result of smooth transition of phase-field variables. Diffusive mass flow in the interface is indicated by $-\rho \mathbf{j}_i$, where \mathbf{j}_i is the volume diffusive flow rate which is only related to the phase-field variable. Hence, the total mass flow rate is $\mathbf{n}_i = \tilde{\rho}_i \mathbf{u} - \rho \mathbf{j}_i$. Cahn and Hilliard [15] assumed that \mathbf{j}_i is proportional to the gradient of the chemical potential, i.e., $\mathbf{j}_i = M_i \nabla \mu_i$, in which M_i and μ_i are the mobility and the chemical potential of fluid i , respectively. The chemical potential is defined in Eq. (7). Substituting the total mass flow rate \mathbf{n}_i into Eq. (2) and recalling the definition of ϕ_i , leads to the following phase-field equations:

$$\frac{\partial \phi_i}{\partial t} + \nabla \cdot (\mathbf{u} \phi_i) = M_i \nabla^2 \mu_i + \frac{\dot{m}_i'''}{\rho_i} \quad i = 1, 2, 3 \quad (3)$$

The chemical potential in Eq. (3) is derived based on free energy functional F for a ternary system defined by [24]

$$F = \int_{\Omega} \left[E_0 + \sum_{i=1}^3 \frac{3}{8} \xi \gamma_i |\nabla \phi_i|^2 \right] d\Omega \quad (4)$$

where E_0 is the bulk free energy defined in Eq. (6), ξ is the interface thickness which is assumed to be the same among all fluids, and γ_i is an auxiliary coefficient related to surface tension coefficients according to [24]

$$\gamma_i = \sigma_{ij} + \sigma_{ik} - \sigma_{jk} \quad \{i, j, k\} \in \{1, 2, 3\} \quad (5)$$

where σ_{ij} is the surface tension coefficient between fluid i and j . The bulk free energy E_0 in Eq. (4) is [24]

$$E_0 = \frac{12}{\xi} \left[\frac{\gamma_1}{2} \phi_1^2 (1 - \phi_1)^2 + \frac{\gamma_2}{2} \phi_2^2 (1 - \phi_2)^2 + \frac{\gamma_3}{2} \phi_3^2 (1 - \phi_3)^2 \right] \quad (6)$$

and the chemical potential of each fluid is given by [21,24]

$$\mu_i = \frac{4\gamma_i}{\xi} \sum_{j \neq i} \left[\frac{1}{\gamma_j} \left(\frac{\partial E_0}{\partial \phi_i} - \frac{\partial E_0}{\partial \phi_j} \right) \right] - \frac{3}{4} \xi \gamma_i \nabla^2 \phi_i \quad i = 1, 2, 3 \quad (7)$$

where $\frac{3}{\gamma_i} = \frac{1}{\gamma_1} + \frac{1}{\gamma_2} + \frac{1}{\gamma_3}$.

We assume that only two of the three fluids take part in phase-change process and the other fluid is neutral in terms of the phase change. In this study, the phase change happens between fluids 1 and 3. Hence, Eq. (3) for each fluid can be written as:

$$\begin{aligned} \frac{\partial \phi_1}{\partial t} + \nabla \cdot (\mathbf{u} \phi_1) &= M_1 \nabla^2 \mu_1 - \frac{\dot{m}'''}{\rho_1} \\ \frac{\partial \phi_2}{\partial t} + \nabla \cdot (\mathbf{u} \phi_2) &= M_2 \nabla^2 \mu_2 \\ \frac{\partial \phi_3}{\partial t} + \nabla \cdot (\mathbf{u} \phi_3) &= M_3 \nabla^2 \mu_3 + \frac{\dot{m}'''}{\rho_3} \end{aligned} \quad (8)$$

Since the phase-field variable are linked together with constraint (1), only the transport equations for fluids 1 and 2 are needed to be solved and the third phase-field variable is obtained via $\phi_3 = 1 - \phi_1 - \phi_2$. The summation of Eq. (8) leads to the divergence of the velocity as follows

$$\nabla \cdot \mathbf{u} = \dot{m}''' \left(\frac{1}{\rho_3} - \frac{1}{\rho_1} \right) \quad (9)$$

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