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Lattice Boltzmann simulation of the thermocapillary flow in an annular two liquid layers system with deformable interface☆

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ABSTRACT

A hybrid model, coupling a finite difference method with a multiple-relaxation-time lattice Boltzmann method, integrating continuum surface force model and phase-field method, for axisymmetric two-phase thermocapillary flow with a deformable interface is developed. Thermocapillary flow, originating from an unbalanced surface tension along the interface of two immiscible liquids in an annular cavity with a horizontal temperature gradient, is simulated numerically. The dynamic behavior of the interface is captured using the phase-field method, and no a priori assumption is made regarding the interface shape and deformation. The continuum surface force model is adopted to add the unbalanced surface tension. The flow field is simulated by multiple-relaxation-time lattice Boltzmann method and both phase-field equation and the energy equation are solved by finite difference method. The dependence of fluid convection and interface deformation on the ratio of physical properties between the two liquid layers is investigated.

1. Introduction

Thermocapillary flow appears in numerous engineering applications with two immiscible liquid layers, for instance, the liquid encapsulation Czochralski (LEC) crystal growth technique [1,2] and floating zone crystal growth [3,4] under microgravity, where the thermocapillary flow dominates convection and therefore heat and mass transfer of the melt. A liquid encapsulant added on melt surface in the LEC growth technique, and the thermocapillary flow in LEC system, is generally much more complicated than in the unencapsulated crystal growth system.

Doi et al. [5] studied theoretically the thermocapillary flow in two immiscible liquids; the flow pattern and the conditions to reduce the flow intensity of the lower layer liquid were investigated. Subsequently, Liu et al. [6] simulated thermocapillary flow with a fixed flat interface assumption and a liquid encapsulation was applied to suppress thermocapillary flow under microgravity. Gupta et al. [7] adopted the finite difference method and domain mapping technique to solve the temperature field and flow field; an effective single-layer model, approximating the flow within the encapsulated layer, was developed. By using a two-dimensional axisymmetric liquid column model, Saghir et al. [8] estimated quantitatively the velocities of thermocapillary flow in three samples of InBi encapsulated in three organic liquids (glycerin, silicone oil, and Krytox). Using a linear perturbative analysis, Madruga et al. [9] studied theoretically the stability of two superposed horizontal liquid layers bounded by two solid planes and subjected to a horizontal temperature gradient, and the existence of three kinds of flow patterns was revealed. Li et al. [10] obtained the asymptotic solution of thermocapillary flow with two-dimensional model for two immiscible liquids with a non-deformable interface in an annular cavity. Someya et al. [11] observed the velocity field with interfacial Marangoni convection by using the particle image velocimetry technique. Koster et al. [12] pointed out that a more detailed investigation on thermocapillary flow in multi-layer fluid system, including the interface deformation, should be considered from the experimental view. However, in these early studies, the dynamical interface deformation is seldom considered in thermocapillary flows because of the unknown interface shape, and the coupling between the interface shape and the convection driving force, i.e. the unbalanced surface tension. In this paper, the technique integrating the phase-field method and continuum surface force (CSF) model is applied to challenge the dynamical interface deformation originating from the unbalanced surface tension driving flow.

So far, lattice Boltzmann method (LBM) has been widely developed to simulate the multiphase flow, and many computational advantages, including easy parallelization and boundary treatment, are exhibited in LBM. The axisymmetric LBM model, incorporating the spatial and velocity dependent source terms into evolution equation to recover N-S

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Nomenclature

f_α	Density distribution function
f^{eq}	Equilibrium distribution function
m_α	Moment
m^{eq}	Equilibrium moment
$\mathbf{e}_\alpha$	Discrete particle speeds
s_α	Relaxation rates
c_p	Heat capacity
$\mathbf{u}$	Velocities
p	Pressure
T	Temperature
$\mathbf{n}$	Interface normal
k	Interface curvature
Re	Reynolds number
Ma	Marangoni number
Ca	Capillary number
Greeks	
σ	Surface tension
φ	Order parameter
κ	Thermal conductivity
ν	Kinematic viscosity
ρ	Density
Subscripts/Superscripts	
α	Discrete speed directions ($\alpha = 0,\ldots,8$)
eq	Equilibrium

equations in cylindrical coordinate, was proposed by Halliday et al. [13]. Subsequently, some modified models, following Halliday's procedure, were developed [14–16]. Zhou [17] introduced a centered scheme for the source terms to simplify the axisymmetric LBM model. The theoretical differences for these LBM axisymmetric models had been discussed in [18] and numerical simulations were also carried out to investigate the accuracy of these models. Chen et al. [19] developed an axisymmetric LBM model from the vorticity-stream equations. Based on the continuous Boltzmann equation in cylindrical coordinates, Guo et al. [20] proposed another approach of axisymmetric kinetic LBM model, in which the gradient was eliminated in source terms. Li et al. [21] presented an improved LBM model with a simplified source term to eliminate velocity gradient for incompressible axisymmetric flows. Recently, the axisymmetric LBM models were widely developed for two-phase flows. The collision of two axisymmetric drops was simulated with two-phase LBM model in [22].The drop spreading on a dry surface was investigated by an axisymmetric two-phase LBM model in [23]. The classical Shen-Chen two-phase model [24] was also extended to axisymmetric flows [25]. Liang et al. [26] developed a phase-field-based two distribution functions LBM model for axisymmetric two-phase isothermal flow.

In this paper, a computational strategy coupling multiple-relaxation-time (MRT) LBM and finite difference method (FDM) is adopted; the technique integrating the phase-field method and continuum surface force (CSF) model is applied to implement the unbalanced surface tension on interface and also track the interface dynamical deformation. The axisymmetric LBM model for the two liquid layers is referred to the works [23,25,27], where Huang developed a phase-field-based hybrid LBM model for simulating axisymmetric isothermal two-phase flow. Thermocapillary flow with deformable interface in an annular pool is simulated, and the influence of the ratio of physical properties on the flow pattern and deformation of the liquid–liquid interface is investigated.

2. Numerical method

In this section, three basic parts of our hybrid two-phase LBM approach for thermocapillary flow with dynamical interface are introduced.

2.1. Axisymmetric LBM for fluids

In LBM, $f_\alpha(\mathbf{x}, t)$ is defined as a particle distribution function at position $\mathbf{x}(r, z)$, time t with velocity $\mathbf{e}_\alpha$. The evolution equation for $f_\alpha(\mathbf{x}, t)$ with a single relaxation time collision model is

$$f_\alpha(\mathbf{x}+\mathbf{e}_\alpha\delta_t, t+\delta_t)-f_\alpha(\mathbf{x},t) = -\frac{1}{\tau}\left[f_\alpha(\mathbf{x},t)-f_\alpha^{eq}(\mathbf{x},t)\right] \tag{1}$$

where $f_\alpha^{eq}(\mathbf{x}, t)$ is the equilibrium distribution function. τ is the single relaxation time and relate to the kinematic viscosity ν. In a two-dimensional nine-velocity (D2Q9) model, the $\mathbf{e}_\alpha$ is

$$\mathbf{e}_\alpha = \begin{cases} (0,\ 0), & \alpha = 0 \\ (\cos[(\alpha-1)\pi/2],\ \sin[(\alpha-1)\pi/2])c, & \alpha = 1-4 \\ (\cos[(2\alpha-9)\pi/4],\ \sin[(2\alpha-9)\pi/4])\sqrt{2}c, & \alpha = 5-8, \end{cases} \tag{2}$$

where $c = \delta_x/\delta_t$ is the lattice velocity. The equilibrium distribution function $f_\alpha^{eq}(\mathbf{x}, t)$ in [28,29] is adopted as

$$f_\alpha^{eq} = \omega_\alpha\left[p + \rho c_s^2\left(\frac{\mathbf{e}_\alpha\cdot\mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_\alpha\cdot\mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u}^2}{2c_s^2}\right)\right], \tag{3}$$

where $c_s^2 = c/3$, and the weight coefficients are

$$\omega_\alpha = \begin{cases} 4/9, & \alpha = 0 \\ 1/9, & \alpha = 1,2,3,4 \\ 1/36, & \alpha = 5,6,7,8 \end{cases}. \tag{4}$$

Next, the external force terms are added directly in the right hand side of the evolution Eq. (1)

$$f_\alpha(\mathbf{x}+\mathbf{e}_\alpha\delta_t, t+\delta_t)-f_\alpha(\mathbf{x},t) = -\frac{1}{\tau}\left[f_\alpha(\mathbf{x},t)-f_\alpha^{eq}(\mathbf{x},t)\right] + \left(1-\frac{1}{\tau}\right)\left\{(\mathbf{e}_\alpha-\mathbf{u})\cdot\left[\nabla\rho c_s^2(\Gamma_\alpha-\Gamma_\alpha(0)) + (\mathbf{F}_s + \mathbf{F}_{1,axis})\Gamma_\alpha\right]-\omega_\alpha F_{0,axis}\right\} \tag{5}$$

where $F_{0,axis}$ is a source term to account for the axisymmetric effect in the continuity equation, and $\mathbf{F}_{1,axis}$ is the parts to mimic the axisymmetric contribution for the momentum equation:

$$\begin{aligned} F_{0,axis} &= c_s^2\frac{\rho u_r}{r} \\ \mathbf{F}_{1,axis} &= (F_{r,axis},\ F_{z,axis}) \\ &= \left(\rho\frac{\nu}{r}\frac{\partial u_r}{\partial r} + \rho\frac{\nu}{r}\frac{\partial u_r}{\partial r} - \rho\frac{u_r u_r}{r} - 2\rho\frac{\nu u_r}{r^2},\ \ \rho\frac{\nu}{r}\frac{\partial u_z}{\partial r} + \rho\frac{\nu}{r}\frac{\partial u_r}{\partial z} - \rho\frac{u_r u_z}{r}\right) \end{aligned} \tag{6}$$

Γ_α is defined as

$$\Gamma_\alpha = \omega_\alpha\left(1 + \frac{\mathbf{e}_\alpha\cdot\mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_\alpha\cdot\mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u}^2}{2c_s^2}\right). \tag{7}$$

Because of the drawback of the instability at low viscosity values in the single relaxation time LBM model, an MRT collision model, improving the numerical stability, was proposed by D'Humières [30]. Lallemand and Luo [31] further developed this model. Premnath [32] derived the continuum equations for multiphase flow from the MRT model through a Chapman–Enskog analysis and demonstrated the computational advantages of the MRT model for multiphase flows.