Physics Letters A 380 (2016) 596–603

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Continuous surface force based lattice Boltzmann equation method for simulating thermocapillary flow

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ARTICLE INFO

Article history:
Received 31 March 2015
Received in revised form 25 November 2015
Accepted 25 November 2015
Available online 27 November 2015
Communicated by R. Wu

Keywords:
Lattice Boltzmann equation
Thermocapillary flow
Continuous surface force

ABSTRACT

In this paper, we extend a lattice Boltzmann equation (LBE) with continuous surface force (CSF) to simulate thermocapillary flows. The model is designed on our previous CSF LBE for athermal two phase flow, in which the interfacial tension forces and the Marangoni stresses as the results of the interface interactions between different phases are described by a conception of CSF. In this model, the sharp interfaces between different phases are separated by a narrow transition layers, and the kinetics and morphology evolution of phase separation would be characterized by an order parameter via Cahn–Hilliard equation which is solved in the frame work of LBE. The scalar convection–diffusion equation for temperature field is resolved by thermal LBE. The models are validated by thermal two layered Poiseuille flow, and two superimposed planar fluids at negligibly small Reynolds and Marangoni numbers for the thermocapillary driven convection, which have analytical solutions for the velocity and temperature. Then thermocapillary migration of two/three dimensional deformable droplet are simulated. Numerical results show that the predictions of present LBE agreed with the analytical solution/other numerical results.

1. Introduction

With the rapid development of the materials and aviation technology, the transport mechanism of interfacial thermodynamics under microgravity/zero gravity or in microfluidic system is one of the hot topics in space science. In the microgravity environment or the microfluidic devices, the effect of gravity is greatly eliminated or even disappeared, then different transports of the interface dynamics are emerged. When the system has a nonuniform temperature distribution, there is a temperature gradient along the interface, which caused to a variation of the surface tension along the interface (the surface tension generally decreases with the increased temperature for most fluids). This variable surface tension force could lead to a viscous stress, which could induce the fluid's motion from a hotter region to a colder region. This phenomenon is known as thermocapillary (Marangoni) convection, which plays a dominant role in microgravity [1] or microfluidic devices [2].

As one of the interesting investigations on thermocapillary convection, the migration of an unconfined spherical droplet/bubble has been investigated extensively [3,1]. In Ref. [3], Young et al. first derived an analytical formulation for the terminal velocity of unconfined non-deformable drop with a linear temperature profile in the creeping flow limit. Since then, there have been numerous subsequent experimental or numerical studies to investigate such phenomenon [1].

As we know, experimental investigations on thermocapillary migration of droplet/bubble are hampered by gravitational effects which tend to mask the thermocapillary effect on terrestrial. To reduce such effects, the drop tower, sounding rockets, and aboard space shuttles are the basic ways to get a short time microgravity environment for investigating thermocapillary convection, while a long time microgravity experiment in space station is an expensive and crucial way, which depended on the aviation program in the whole world [4]. Although experimental investigations could help to understand the phenomena of thermocapillary flows in microgravity/microfluidic devices, it is still difficult to precisely measure the local temperature and flow fields during the transport process of a droplet/bubble.

On the other hand, numerical method has been viewed as a scientific method for the fluid dynamics, which has been successfully applied to the thermocapillary flows [5–12]. However, an efficient and precise description of phase interaction or its interfacial dynamics model is still a challenging task. In the literature, there are generally two clarifications of numerical methods for simulating thermocapillary flow: one is single phase Navier–Stokes equations

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http://dx.doi.org/10.1016/j.physleta.2015.11.033
0375-9601/

(NSE) based numerical method [5–8]; another is the two phase NSE based numerical method [9–12]. In the former method, the physical problem is mainly focused on dynamics of one phase, and the thermocapillary effect is included by interface boundary conditions, which is usually used to some simplified thermocapillary convection problems. In the latter one, the detailed physical phenomena of the interface dynamics in both phases could be observed, and there is no need to implement the interface boundary conditions throughout the computation except for the sharp interface method. It is well understood that the interface dynamics of the two phase flow is just the result of molecular interactions between different phases. Thus, if we could design a model that could correctly describe such interaction process at microscopic level, the corresponding interface dynamics could be obtained at macroscopic level. The lattice Boltzmann method (LBE) is just one of the mesoscopic methods, which could be applied to model such interaction process [13,14,11,12,15]. In Refs. [11,12], the authors applied the color-fluid and phase field based LBE to model the CSF, while a LBE is used to temperature field with equal density [11] and a finite difference scheme is applied to solve the internal energy equation with unequal density [12], the numerical simulations showed that both schemes could give satisfied results.

In this paper, we will extend previous continuous surface force (CSF) LBE to the thermocapillary flow, and the effect of the Marangoni force is included through the CSF formulation [16,11]. The evolution of interface is governed by the Cahn–Hilliard equation (CHE), which is solved by LBE, and a thermal LBE is derived from the kinetic theory for solving the scalar convection–diffusion energy equation. The rest of this paper is organized as follows. In Sec. 2, a continuous surface force formulation of LBE model is presented, and a LBE model for temperature field is proposed in Sec. 3, then some numerical simulations are conducted to validate the models in Sec. 4, and finally a brief conclusion is given in Sec. 5.

2. LBE with continuous surface force

In general, surface tension is a function of local temperature in thermal multiphase system, so the effect of tangential gradient of the surface tension should be included in the CSF formulation, and the governing equation for the momentum could be written as

$$\partial_t(\rho \boldsymbol{u}) + \nabla\cdot(\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla\cdot \boldsymbol{S} + \boldsymbol{F}, \tag{1}$$

where ρ is the fluid density, $\boldsymbol{u}$ is the velocity, p is the hydrodynamic pressure, $\boldsymbol{S}$ is the viscous stress term and the interface force $\boldsymbol{F}$ in Eq. (1) is given as [16]

$$\boldsymbol{F} = -\sigma\kappa\delta\boldsymbol{n} + \nabla_s\sigma\delta \tag{2}$$

where σ is the surface tension, κ is the total curvature, δ is a regularized delta function, $\boldsymbol{n}$ is the outward pointing unit normal vector, and $\nabla_s = (\boldsymbol{I} - \boldsymbol{nn})\cdot\nabla$ is the surface gradient operator. The first term on the right hand side of Eq. (2) is the normal surface tension force, and the second is the tangential force which is the result of the nonuniform surface tension. Alternately, one may write $\boldsymbol{F}$ in a stress formulation

$$\boldsymbol{F} = \nabla\cdot[(\boldsymbol{I} - \boldsymbol{nn})\sigma\delta] \tag{3}$$

With this interface force formulation in Eq. (2), a diffuse interface formulation of $\boldsymbol{F}$ could be written as

$$\boldsymbol{F} = (-\sigma\nabla\cdot\boldsymbol{nn} + \nabla_s\sigma)\epsilon\alpha|\nabla c|^2 \tag{4}$$

where $\boldsymbol{n} = \nabla c/|\nabla c|$ with c the order parameter, ϵ is a small parameter related to the interface thickness and α is a normalized constant to be determined later. Comparing with Eqs. (2) and (4), the curvature κ relates to the unit normal vector $\boldsymbol{n}$ as $\kappa = \nabla\cdot\boldsymbol{n}$ and the regularized delta function δ relates to the order parameter as $\delta = \epsilon\alpha|\nabla c|^2$.

In thermocapillary flow, the flow is driven by surface tension force which is a function of the temperature. For simplicity, we assume that the relation of the surface tension to the temperature is a linear relation in present work

$$\sigma = \sigma_0 + \sigma_T(T - T_0), \tag{5}$$

where σ_0 is the surface tension at the reference temperature T_0, $\sigma_T = \partial\sigma/\partial T$ is the rate of change of interfacial tension with temperature, and T is local temperature.

With the formulations of Eqs. (4) and (5), we can derive a similar incompressible LBE model with CSF for the fluid flow [13–15]

$$\begin{aligned} &f_i(\boldsymbol{x} + \boldsymbol{\xi}_i\delta t, t + \delta t) - f_i(\boldsymbol{x}, t) \\ &\quad = -\omega(f_i - f_i^{(eq)}) + \delta t(1 - \tfrac{\omega}{2})[\boldsymbol{F}\cdot(\boldsymbol{\xi}_i - \boldsymbol{u})\Gamma_i(\boldsymbol{u}) \\ &\qquad + (\boldsymbol{\xi}_i - \boldsymbol{u})\cdot\nabla(\rho c_s^2)(\Gamma_i(\boldsymbol{u}) - \Gamma_i(0))], \end{aligned} \tag{6}$$

where f_i is the density distribution function, $\boldsymbol{\xi}_i$ is the molecular velocity, δt is the time step, $\omega = 1/\tau_f$ is the relaxation rate with τ_f the relaxation time, and $f_i^{(eq)}$ is equilibrium density distribution function which is given as

$$f_i^{(eq)} = \omega_i\left[p + \rho c_s^2\left(\frac{\boldsymbol{\xi}_i\cdot\boldsymbol{u}}{c_s^2} + \frac{1}{2}\left((\frac{\boldsymbol{\xi}_i\cdot\boldsymbol{u}}{c_s^2})^2 - \frac{\boldsymbol{u}^2}{c_s^2}\right)\right)\right], \tag{7}$$

and $\Gamma_i(\boldsymbol{u})$ is given as

$$\Gamma_i(\boldsymbol{u}) = \omega_i\left\{1 + \frac{\boldsymbol{\xi}_i\cdot\boldsymbol{u}}{c_s^2} + \frac{1}{2}\left[\left(\frac{\boldsymbol{\xi}_i\cdot\boldsymbol{u}}{c_s^2}\right)^2 - \frac{\boldsymbol{u}^2}{c_s^2}\right]\right\}, \tag{8}$$

where ω_i is the weight coefficient depending on the number of discrete velocity $\boldsymbol{\xi}_i$, c_s is sound speed. The dynamic pressure and velocity defined by the velocity moments of the density distribution function are given by

$$p = \sum_i f_i + \frac{\delta t}{2}\boldsymbol{u}\cdot\nabla\rho c_s^2, \qquad \rho c_s^2\boldsymbol{u} = \sum_i \boldsymbol{\xi}_i f_i + \frac{\delta t}{2}\boldsymbol{F} \tag{9}$$

Through the Chapman–Enskog (CE) analysis, the following governing equations could be obtained

$$\nabla\cdot\boldsymbol{u} = 0, \tag{10}$$

$$\partial_t(\rho\boldsymbol{u}) + \nabla\cdot(\rho\boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla\cdot\boldsymbol{S} + \boldsymbol{F}, \tag{11}$$

where the viscous stress $\boldsymbol{S} = \eta(\nabla\boldsymbol{u} + \boldsymbol{u}\nabla)$ with viscosity $\eta = \rho c_s^2(\tau_f - 1/2)\delta t$.

In the phase field theory, the kinetics and morphology evolution of phase separation is characterized by CHE via an order parameter c. It is usually used to identify the two phase region, where $c = c_1$ occupied by fluid 1, and $c = c_2$ occupied by fluid 2. The mixing free energy of such fluid for the isothermal system without the solid boundaries can be written as

$$E = \int[E_0 + \frac{\epsilon^2}{2}|\nabla c|^2]d\Omega,$$

where E_0 is a bulk energy, which is related to the bulk chemical potential by $\mu_0 = \partial_c E_0$. In the phase field theory, E_0 can be approximated by $E_0(c) = \beta(c - c_1)^2(c - c_2)^2$ with β a constant coefficient, c_1 and c_2 respectively the corresponding order parameter at fluid 1 and fluid 2. For planar interface at $z = 0$ in an equilibrium system, the distribution of the order parameter has the following analytical solution

$$c(z) = \frac{c_1 + c_2}{2} + \frac{c_1 - c_2}{2}tanh(\frac{z}{2\sqrt{2}\epsilon}),$$