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A lattice Boltzmann method for axisymmetric thermocapillary flows

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ABSTRACT

In this work, we develop a two-phase lattice Boltzmann method (LBM) to simulate axisymmetric thermocapillary flows. This method simulates the immiscible axisymmetric two-phase flow by an improved color-gradient model, in which the single-phase collision, perturbation and recoloring operators are all presented with the axisymmetric effect taken into account in a simple and computational consistent manner. An additional lattice Boltzmann equation is introduced to describe the evolution of the axisymmetric temperature field, which is coupled to the hydrodynamic equations through an equation of state. This method is first validated by simulations of Rayleigh–Bénard convection in a vertical cylinder and thermocapillary migration of a deformable droplet at various Marangoni numbers. It is then used to simulate the thermocapillary migration of two spherical droplets in a constant applied temperature gradient along their line of centers, and the influence of the Marangoni number (Ca), initial distance between droplets (S_0), and the radius ratio of the leading to trailing droplets (Λ) on the migration process is systematically studied. As Ma increases, the thermal wake behind the leading droplet strengthens, resulting in the transition of the droplet migration from coalescence to non-coalescence; and also, the final distance between droplets increases with Ma for the non-coalescence cases. The variation of S_0 does not change the final state of the droplets although it has a direct impact on the migration process. In contrast, Λ can significantly influence the migration process of both droplets and their final state: at low Ma, decreasing Λ favors the coalescence of both droplets; at high Ma, the two droplets do not coalesce eventually but migrate with the same velocity for the small values of Λ, and decreasing Λ leads to a shorter equilibrium time and a faster migration velocity.

1. Introduction

Thermocapillary convection is a phenomenon of fluid movement that arises as a consequence of the variation of interfacial tension at a fluid–fluid interface caused by temperature differences. It can be employed as a mechanism for driving the motion of droplets and bubbles immersed in a second fluid. For most fluids, the interfacial tension decreases with increasing temperature, and the induced thermocapillary stresses (also called Marangoni stresses) lead to the migration of droplets or bubbles from the regions of low temperature, where the interfacial tension is high, to the warmer regions, where the interfacial tension is low. The thermocapillary migration of droplets and bubbles plays an important role in various industrial applications involving microgravity or microfluidic devices, where bulk phenomena can be negligible in comparison with interfacial effects due to large surface-to-volume ratio and low Reynolds number. To date, it has attracted an increasing amount of research interest worldwide along with the progress of human space exploration and microfluidic technologies.

The study on the thermocapillary migration of droplets or bubbles dates back to the pioneering work of Young et al. [1], who derived an analytical expression for the terminal migration velocity of an isolated spherical droplet in a constant temperature gradient by assuming that the convective transport of momentum and energy are negligible. Since then, extensive works on this subject have been conducted theoretically, experimentally and numerically, and most of them have been summarized in the review book by Subramanian and Balasubramaniam [2] as well as in the recent article by Yin and Li [3]. However, it is still challenging to conduct precise experimental measurements of the local temperature and flow fields during the migration process of droplets. Theoretical study based on the method of reflections has been used for predicting the motion of two well-separated droplets at an arbitrary orientation relative to the line of droplet centers [4]. Unfortunately, it is restricted to ideally spherical droplets and is unable to describe the deformation and coalescence of droplets.

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Numerical modelling and simulations can complement theoretical and experimental studies, providing an efficient pathway to enhance our understanding of the thermocapillary migration and interaction of droplets.

A variety of numerical methods have been proposed to simulate thermocapillary flows with deformed interfaces, and they can roughly be divided into two categories: one is the interface-tracking method, which uses the Lagrangian approach to explicitly represent the interface, such as the front-tracking method [5,3], boundary-integral method [6], and immersed-boundary method [7]; and the other is the interface-capturing method, which uses an indicator function to implicitly represent the interface in an Eulerian grid, such as the volume-of-fluid (VOF) method [8], and level-set (LS) method [9]. However, the interface-tracking methods are not suitable for dealing with interface breakup and coalescence, because the interface must be manually ruptured based upon some *ad hoc* criteria. The VOF and LS methods require interface reconstruction or reinitialization to represent or correct the interface, which may be complex or unphysical. Physically, the interface and its dynamical behavior are the natural consequence of microscopic interactions among fluid molecules. Thus, mesoscopic level methods may be better suited to simulate complex interfacial dynamics in a multiphase system.

The lattice Boltzmann method (LBM) is known to be capable of modeling interfacial interactions while incorporating fluid flow as a system feature. It is a pseudo-molecular method based on particle distribution functions that performs microscopic operations with mesoscopic kinetic equations and reproduces macroscopic behavior. The LBM has several advantages over traditional CFD methods such as the ability to be programmed on parallel computers and the ease in dealing with complex boundaries [10]. Besides, its kinetic nature provides many of the advantages of molecular dynamics, making the LBM particularly useful for simulating multiphase, multicomponent flows. A number of multiphase, multicomponent models have been proposed in the LBM community, and they can be classified into four major types: color-gradient model [11], phase-field-based model [12–14], interparticle-potential model [15], and mean-field theory model [16]. These models have gained great success in simulating multiphase flow problems with a constant interfacial tension [17,10]. Based on the color-gradient model, we proposed the first LBM model to simulate thermocapillary flows, through which we for the first time demonstrated numerically that the droplet manipulation can be achieved through the thermocapillary forces induced by the laser heating [18]. This model was later extended to deal with fluid-surface interactions [19]. In addition, we developed two phase-field-based thermocapillary models with one focusing on high-density-ratio two-phase flows [20] and the other on modelling fluid-surface interactions [21]. The thermocapillary color-gradient model inherits a series of advantages of the model by Halliday and his coworkers [22,23], such as low spurious velocities, high numerical accuracy, strict mass conservation for each fluid and good numerical stability for a broad range of fluid properties, and its three-dimensional (3D) version is capable of simulating the axisymmetric thermocapillary migration of two spherical droplets subject to a constant temperature gradient in an infinite domain, as considered in this work. Such a treatment, however, does not take the advantage of the axisymmetric property of the thermal flow and usually needs large computational costs. Alternatively, one can develop an axisymmetric version of the color-gradient LBM that allows for the solution of thermocapillary flows at the computational cost of a 2D simulation.

In this work, an axisymmetric two-phase LBM, developed on the basis of the Cartesian thermocapillary model of Liu et al. [18], is presented to simulate thermocapillary flows. This method simulates the axisymmetric two-phase flow through a multiple-relaxation-time (MRT) color-gradient model, in which the single-phase collision, perturbation and recoloring operators are all presented with the axisymmetric effect taken into account in a simple and computational consistent manner. An additional lattice Boltzmann equation is also introduced to describe the evolution of the axisymmetric temperature field, which is coupled to the interfacial tension by an equation of state. The capability and accuracy of this method are first tested by two benchmark cases, i.e. Rayleigh–Bénard convection in a vertical cylinder and thermocapillary migration of a deformable droplet at various Marangoni numbers. It is then used to simulate the thermocapillary migration of two spherical droplets subject to a constant temperature gradient along their line of centers, in which the influence of the Marangoni number, initial distance between the centers of two droplets, and the radius ratio of the leading to trailing droplets on the migration process is systematically investigated. To the best of our knowledge, the present method is the first axisymmetric thermocapillary LBM, and the study on the thermocapillary migration and interaction can provide useful suggestions and guidance for the design and optimization of the future space experiments.

2. Numerical method

In this section, we present an axisymmetric version of the color-gradient LBM for thermocapillary flows, and it is developed on the basis of our previous Cartesian model [18], in which the capillary and Marangoni forces are both modeled using the concept of the continuum surface force [24], and the temperature is solved by a passive scalar approach and coupled with the flowfield through an equation of state. In the color-gradient LBM, two sets of distribution functions f_i^R and f_i^B are introduced to represent the "red" and "blue" fluids. The total distribution function is defined by $f_i = f_i^R + f_i^B$, which undergoes a collision step as

$$f_i^{\dagger}(\mathbf{x}, t) = f_i(\mathbf{x}, t) + \Omega_i(\mathbf{x}, t) + \Phi_i, \tag{1}$$

where $f_i(\mathbf{x}, t)$ is the total distribution function in the ith velocity direction at the position $\mathbf{x}$ and time t, $f_i^{\dagger}$ is the post-collision distribution function, Ω_i is the single-phase collision operator, and Φ_i is the forcing term. The single-phase collision operator is designed to recover the correct macroscopic equations of incompressible axisymmetric flows in each single-phase region. For the axisymmetric flows with an axis in the z-direction, the single-phase collision operator is given by [25,26]

$$\Omega_i(\mathbf{x}, t) = -\sum_j (\mathbf{M}^{-1}\mathbf{S}\mathbf{M})_{ij}\left[f_j(\mathbf{x}, t) - f_j^{eq}(\mathbf{x}, t)\right] + \delta_t h_i(\mathbf{x} + \mathbf{e}_i\delta_t/2, t + \delta_t/2), \tag{2}$$

which adopts the MRT model [27] instead of the Bhatangar–Gross–Krook (BGK) approximation in order to enhance the numerical stability and reduce unphysical spurious velocities. In the above equation, f_i^{eq} is the equilibrium distribution functions of f_i; $\mathbf{M}$ is a transformation matrix; $\mathbf{S}$ is a diagonal relaxation matrix; and h_i is a source term defined at the position $(\mathbf{x} + \mathbf{e}_i\delta_t/2)$ and time $(t + \delta_t/2)$, where δ_t is the time step, and $\mathbf{e}_i$ is the lattice velocity in the ith direction. For the two-dimensional 9-velocity (D2Q9) model, $\mathbf{e}_i$ is defined as $\mathbf{e}_0 = (0, 0), \mathbf{e}_{1,3} = (\pm c, 0), \mathbf{e}_{2,4} = (0, \pm c), \mathbf{e}_{5,7} = (\pm c, \pm c)$, and $\mathbf{e}_{6,8} = (\mp c, \pm c)$, where $c = \delta_x/\delta_t$ with δ_x being the lattice spacing.

The equilibrium distribution function is obtained by a second order Taylor expansion of Maxwell–Boltzmann distribution with respect to the local fluid velocity $\mathbf{u}$:

$$f_i^{eq} = \rho w_i\left[1 + \frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_i \cdot \mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u}^2}{2c_s^2}\right], \tag{3}$$