Journal of Computational Physics 280 (2015) 37–53

Contents lists available at ScienceDirect

Journal of Computational Physics

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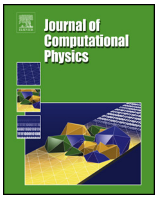

Modelling thermocapillary migration of a microfluidic droplet on a solid surface

Haihu Liu [a,b,*], Yonghao Zhang [b]

[a] School of Energy and Power Engineering, Xi'an Jiaotong University, 28 West Xianning Road, Xi'an 710049, China
[b] James Weir Fluids Laboratory, Department of Mechanical & Aerospace Engineering, University of Strathclyde, Glasgow G1 1XJ, UK

ARTICLE INFO

Article history:
Received 7 January 2014
Received in revised form 13 July 2014
Accepted 2 September 2014
Available online 28 September 2014

Keywords:
Thermocapillary migration
Lattice Boltzmann method
Multiphase flow
Wetting boundary condition
Microfluidics
Droplet dynamics

ABSTRACT

A multiphase lattice Boltzmann model is developed to simulate immiscible thermocapillary flows with the presence of fluid–surface interactions. In this model, interfacial tension force and Marangoni stress are included by introducing a body force term based on the concept of continuum surface force, and phase segregation is achieved using the recolouring algorithm proposed by Latva-Kokko and Rothman. At a solid surface, fluid–surface interactions are modelled by a partial wetting boundary condition that uses a geometric formulation to specify the contact angle, and a colour-conserving boundary closure scheme to improve the numerical accuracy and suppress spurious velocities at the contact line. An additional convection–diffusion equation is solved by the passive scalar approach to obtain the temperature field, which is coupled to the hydrodynamic equations through an equation of state. This model is first validated by simulations of static contact angle and dynamic capillary intrusion process when a constant interfacial tension is considered. It is then used to simulate the thermocapillary migration of a microfluidic droplet on a horizontal solid surface subject to a uniform temperature gradient. We for the first time demonstrate numerically that the droplet motion undergoes two different states depending on the surface wettability: the droplet migrates towards the cooler regions on hydrophilic surfaces but reverses on hydrophobic surfaces. Decreasing the viscosity ratio can enhance the intensity of thermocapillary vortices, leading to an increase in migration velocity. The contact angle hysteresis, i.e., the difference between the advancing and receding contact angles, is always positive regardless of the contact angle and viscosity ratio. The contact angle hysteresis and the migration velocity both first decrease and then increase with the contact angle, and their minimum values occur at the contact angle of 90 degrees.

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 gradients. It has been known as a mechanism for driving the motion of droplets and bubbles immersed in the second fluid since the pioneering work of Young et al. [1]. For most fluids interfacial tension is a decreasing function of temperature, and this leads to the movement of droplets or bubbles

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[*] Corresponding author at: James Weir Fluids Laboratory, Department of Mechanical & Aerospace Engineering, University of Strathclyde, Glasgow G1 1XJ, UK.

E-mail address: haihliu@gmail.com (H. Liu).

http://dx.doi.org/10.1016/j.jcp.2014.09.015
0021-9991/

suspended in a bulk fluid from the regions of lower temperature to the warmer regions; such a subject has been studied extensively due to its importance in space material processing and many other engineering and scientific applications under microgravity conditions where sedimentation and gravity-driven convection are largely eliminated [2]. Over the last decade or so, attention has been focused on using thermocapillary forces to manipulate the motion and dynamic behaviour of droplets or bubbles in microfluidic devices, where bulk phenomena can be negligible in comparison with interfacial effects due to large surface-to-volume ratio and low Reynolds number. Thermocapillary actuation is advantageous over convectional hydrodynamic stress, electrohydrodynamic force, and magnetic force methods for droplet and bubble manipulations, as it can be generated easily by means of substrate embedded microheaters [3,4] or by localized laser heating [5,6] that allows contactless, reconfigurable, and real-time control of multiple droplets without the need for any special microfabrication or moving parts. To date, the thermocapillary force has been combined with geometry of the microchannel to realise various droplet manipulations including mixing, sorting, fission, fusion, sampling and switching [7,8].

Unlike droplets suspended in a carrier fluid, droplets are typically in touch with channel walls in microfluidic devices. The confinement and wettability of channel walls would quantitatively or qualitatively modify the physics of thermocapillary migration in a microfluidic channel [5,9]. For example, it was observed that a liquid droplet placed on a horizontal solid surface can move toward cooler regions [10], as opposed to that in an unbounded flow condition. There have been a number of experimental studies investigating the migration of a liquid droplet on a solid surface induced by thermal gradients [11–15]. However, it is still very difficult to conduct precise experimental measurements of the local temperature and flow fields during the migration process of a droplet. Theoretical studies based on a lubrication approximation have been used for analyzing the migration velocity of a droplet with sufficiently small aspect ratio (defined by the maximum height of the droplet to its length) induced by thermocapillary force [16,17,10,18]. Unfortunately, they are unable to solve the transient thermocapillary migration of a spherical cap droplet with a large contact angle due to the limitation of lubrication approximation. Numerical modelling and simulations can complement theoretical and experimental studies, providing an efficient pathway to enhance our understanding of thermocapillary migration of droplets in a microchannel.

Computational modelling of thermocapillary flows with fluid–surface interactions is a challenging task. Discretization errors in computation of interfacial forces may generate unphysical spurious velocities that can cripple the velocity field in the whole computational domain. Minimization of spurious velocities at the interface still remains a major challenge for many numerical models and algorithms. In addition, contact line dynamics is still a challenging problem that has not been fully solved because of its inherent multiscale nature [19]. Finally, due to strong dependence of interfacial tension on temperature, temperature fluctuations result in non-uniform interfacial tension forces and Marangoni stresses that affect the velocity field near the interface, which in turn alters the interfacial temperature distribution through the induced interfacial flows. Although traditional CFD (computational fluid dynamics) methods such as volume-of-fluid [20,21] and level-set methods [22,23] have been extensively used for simulating various multiphase flow problems, they suffer from numerical instability at the interface region when the interfacial tension becomes a dominant factor in microdroplet behaviour [24]. Moreover, an empirical slip model with slip length at the molecular scale has to be introduced in these methods to avoid stress singularities at the moving contact line [25]. Microscopically, the interface between different phases and the contact line dynamics on the solid surface are due to interparticle interactions [26]. Thus, mesoscopic level models are expected to describe more accurately the multiscale thermocapillary flows in a confined microfluidic device.

The lattice Boltzmann (LB) method has become a promising alternative to traditional CFD methods for simulating complex fluid flow problems. It is a pseudo-molecular method based on particle distribution functions that performs microscopic operations with mesoscopic kinetic equations and reproduces macroscopic behaviour [27]. Its mesoscopic kinetic nature offers many of the advantages of molecular dynamics, making LB method particularly suited for modelling multiphase, multicomponent flows. A number of multiphase, multicomponent models have been proposed in the LB community, which can be classified into four major types: colour-fluid model [28–31], phase-field-based model [32–34], interparticle-potential model [35–37], and mean-field theory model [38]. These models have shown great success in modelling multiphase flow problems with a constant interfacial tension [39]. Based on the colour-fluid model, we recently proposed the first LB model to simulate thermocapillary flows, through which we first numerically demonstrate that the micro-droplet manipulation can be achieved through the thermocapillary forces induced by the laser heating [40]. Later, we developed two phase-field-based thermocapillary models with one focusing on high-density-ratio two-phase flows [41] and the other on modelling fluid–surface interactions [9]. Although the thermocapillary colour-fluid model inherits a series of advantages of the model by Halliday and his coworkers [42,29], such as low spurious velocities, high numerical accuracy and strict mass conservation for each fluid, it can only simulate thermocapillary flows with droplets suspended in a carrier fluid, away from the wall boundary.

In this paper, we present a colour-fluid LB model to simulate immiscible thermocapillary flows with the presence of fluid–surface interactions. A two-phase collision operator based on the concept of a continuum surface force (CSF) [43] is used to model the interfacial tension force and Marangoni stress, and the recolouring operator proposed by Latva-Kokko and Rothman [44] is introduced to maintain the interface between two fluids. An additional convection–diffusion equation is solved by a passive-scalar approach [45] to obtain the temperature field, which is coupled to the interfacial tension by an equation of state. At the solid surface, a previously developed wetting boundary condition [46] is incorporated into the model to account for fluid–surface interactions, in which the contact angle is enforced through a geometric formulation [47] and the colour-conserving boundary closure scheme [48] is applied to improve the numerical accuracy and suppress spurious currents at the contact line. The capability and accuracy of this model are first tested by two benchmark cases with