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Numerical study of gravity-driven droplet displacement on a surface using the pseudopotential multiphase lattice Boltzmann model with high density ratio

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ABSTRACT

Gravity-driven displacement of a droplet on a grooved surface is studied using the Shan and Chen's pseudopotential multiphase lattice Boltzmann (LB) model allowing a high density ratio between the gas and liquid phases. To verify and validate the multiphase LB model, we find good agreement of the LB simulations with the pressure difference over a droplet described by Laplace's law, as well as with the dynamic capillary intrusion process obtained by Washburn's law. The equilibrium contact angle of a droplet on a smooth horizontal surface is studied as a function of the wettability, finding good agreement with an empirical scheme obtained with Young's equation. The dynamic behavior of a droplet moving down a vertical surface under different gravitational forces is studied. On a vertical wall, the liquid droplet reaches a terminal velocity, which value depends on the wettability of the surface and strength of the gravitational force. When a hydrophilic groove is introduced along the surface, the droplet shows a complex behavior and, depending on the height of the groove, different patterns and mechanisms of the liquid filling the groove are observed. For small groove heights, the droplet totally fills in the groove. At certain groove height, a liquid bridge is formed between top and bottom surfaces dragging most liquid onto the bottom surface. At increasing height, this liquid bridge is broken, and liquid can be dragged into the groove by adhesion force. At high groove heights, the droplet breaks up in smaller droplets dripping from the top surface onto the bottom surface, and only a small amount of liquid remains in the groove. When the wettability of the groove or surface is changed, the liquid filling behavior changes notably. For a hydrophobic surface, but hydrophilic groove, the groove is filled partly by the liquid, while, for the opposite condition, a hydrophobic groove in a hydrophilic wall, the droplet runs into the groove, but the liquid is again dragged out and no filling of the groove occurs.

1. Introduction

The study of the displacement of a droplet on a surface, such as the deposit and runoff of a droplet on surfaces of different roughness or in the presence of grooves, is of common interest. Applications are found in inkjet printing, coating, etc. Such multiphase phenomena can be studied solving the Navier–Stokes equations using computational fluid dynamics (CFD), combined with front tracking or front capturing methods, among which the Volume of Fluid (VOF) [1] and the level set method [2] are widely adopted. These front tracking or front capturing methods are based on an additional calculation step to track the phase interface. It is known that VOF may introduce some numerical diffusion and requires more complex algorithms, making it less convenient for three-dimensional problems [1]. The level set method is simpler to apply and can handle sharp interfaces in three-dimensional cases. However, level set method may show mass conservation problems near interfaces [2]. When these methods are applied on complex geometries or small scale problems, these limitations can become particularly significant.

The lattice Boltzmann method (LBM), which is based on microscopic models and mesoscopic equations, is considered an attractive numerical alternative for solving multiphase phenomena

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[3,4]. The kinetic nature of the LBM allows representing the microscopic interactions between different fluids, thereby facilitating the automatic tracking of the fluid interfaces in a multiphase system [5,6]. Also fluid–solid interactions can be implemented conveniently in the LBM without introducing additional complex kernels [7]. Owing to its constitutive versatility, the LBM has developed into a powerful technique for simulating transport processes, and is particularly successful in modelling transport processes involving interfacial dynamics and complex geometries, such as multiphase flow in porous media [3,4,8]. Several LB models have been developed for multiphase flow simulation including the color-gradient based LB method by Gunstensen et al. [9], the free-energy model by Swift et al. [10], the mean-field model by He et al.[11] and the pseudopotential model by Shan and Chen [5,6]. Among them, the pseudopotential model, to the best of the authors' knowledge, is the most widely used LB multiphase model due to its simplicity and versatility. This model represents microscopic molecular interactions at mesoscopic scale using a pseudopotential (also often called effective mass) depending on the local density [5,6]. With such interactions, a single component fluid spontaneously segregates into a high and low density phases (e.g. liquid and gas), when the interaction strength (or the temperature) is under the critical point [5,6]. The automatic phase separation is an attractive characteristic of the pseudopotential model, as the phase interface is no longer a mathematical boundary and no explicit interface tracking or interface capturing technique is needed. The location of the phase interface is characterized through monitoring of the jump of the fluid density from gas to liquid. The pseudopotential model captures the essential elements of fluid behavior, namely it follows a non-ideal equation of state (EOS) and incorporates a surface tension force. Due to its remarkable computational efficiency and clear representation of the underlying microscopic physics, this model has been used as an efficient technique for simulating and investigating multiphase flow problems, particularly for these flows with complex topological changes of the interface, such as deformation, coalescence and breakup of the fluid phase, or fluid flow in complex geometries [12]. Recently, Chen et al. [8] thoroughly reviewed the theory and application of the pseudopotential model, and we refer to their paper for more details.

The pseudopotential model has been used to simulate droplet displacement on surfaces. Kang et al. [13] investigated a two-dimensional droplet flowing down a channel with different Bond numbers. The Bond number is the dimensionless number representing the ratio between gravitational force and surface tension. The effects of surface wettability, droplet size and density, and viscosity ratio were studied. Mazloomi and Moosavi [14] simulated the runoff of a gravity-driven liquid film over a vertical surface displaying U- and V-shaped grooves or mounds. Their results showed that each groove and mound has a critical width for successful coating or covering with fluid. If the width of a groove is larger than a critical width, the grooves and surface are fully coated. This critical width depends on the capillary number, contact angle and groove width and height. On surfaces with several grooves of the same geometry, there exists a critical distance between grooves for full coating of the groove. The study provided a relationship between critical distance, contact angle and capillary number. However, their explanation of the interactive force balance to control liquid displacement on a vertical surface was found to be insufficient. Azwadi and Witrib [15] investigated the dynamic behavior of droplets with respect to contact angle, Bond number and tilting of the surface. Li et al. [16] studied the deformation and breakup of a droplet in a channel with a solid obstacle. They investigated droplet breakup and deformation considering different obstacle shapes, wettability, viscous ratio and Bond number. In all works, the displacement of an immiscible fluid with a low density ratio between liquid and gas, usually equal to 1, is investigated. We finally mention the work of Huang et al. [17] who studied, for high density ratio, the droplet motion inside a grooved channel considering different surface wettability, surface tension, tilt angles and geometries. However this multiphase LB model is different to the approach presented in this paper.

The present study considers a single component multiphase problem with high density ratio between liquid and gas. The displacement of a two-dimensional droplet, flowing down a grooved surface due to gravitational force, is investigated using the Shan and Chen's pseudopotential LB model. In most LB models, it is difficult to achieve a high density ratio between the two phases. Increasing the density ratio results commonly in large spurious currents and makes the simulation unstable. Therefore, most LB modelling focused on multiphase problems with a density ratio of less than 10. In this paper, the Carnahan–Starling (C–S) equation of state (EOS) [18] is combined with a force scheme based on the exact-different method (EDM) [19] for a high density ratio problem guaranteeing low spurious currents and numerical stability. The influence of different groove geometry, wettability and tilt angles of the surface is investigated in detail.

The paper is organized as follows: in Section 2, we describe the pseudopotential multiphase LB model with the C–S EOS; in Section 3, validation cases are presented; the computational set-up of the gravity-driven droplet on a grooved surface and results are presented in Section 4; and finally in Section 5, conclusions are drawn.

2. Numerical method

The LBM considers flow as a collective behavior of pseudoparticles residing on a mesoscopic level, and solves the Boltzmann equation using a small number of velocities adapted to a regular grid in space. The LBM has been successfully applied to a wide range of complex transport problems, such as porous flow [7], multiphase flow [13], particle flow [20] and reactive transport processes [21–23]. In the LB equation, fluid motion is represented by a set of particle distribution functions. The evolution equation, which is based on the Bhatnagar–Gross–Krook (BGK) collision operator, is written as

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

where $f_\alpha(\mathbf{x},t)$ is the density distribution function and $f_\alpha^{eq}(\mathbf{x},t)$ is the equilibrium distribution function. $\mathbf{x}$ denotes the position, t is the time and α is the lattice direction. A relaxation time τ is introduced, which relates to the kinematic viscosity as $\upsilon = c_s^2(\tau - 0.5)\triangle t$. The lattice sound speed c_s is equal to $c/\sqrt{3}$, where c the lattice speed is equal to $\triangle x/\triangle t$, with the grid spacing $\triangle x$ and the time step $\triangle t$. In the LBM, both the grid spacing and time step are set equal to 1. For the D2Q9 lattice model with nine velocity directions at a given point in two-dimensional space, the discrete velocity $\mathbf{e}_\alpha$ is given by

$$\mathbf{e}_\alpha = \begin{cases} (0,0), & \alpha = 0; \\ \left(\cos\left[\frac{(\alpha-1)\pi}{2}\right], \sin\left[\frac{(\alpha-1)\pi}{2}\right]\right), & \alpha = 1,2,3,4; \\ \sqrt{2}\left(\cos\left[\frac{(\alpha-5)\pi}{2} + \frac{\pi}{4}\right], \sin\left[\frac{(\alpha-5)\pi}{2} + \frac{\pi}{4}\right]\right), & \alpha = 5,6,7,8. \end{cases} \tag{2}$$

The equilibrium distribution function for the D2Q9 lattice model is of the form

$$f_\alpha^{eq} = w_\alpha \rho \left[1 + \frac{3}{c^2}(\mathbf{e}_\alpha \cdot \mathbf{u}) + \frac{9}{2c^4}(\mathbf{e}_\alpha \cdot \mathbf{u})^2 - \frac{3}{2c^2}\mathbf{u}^2\right] \tag{3}$$

where the weighting factors w_α are given by

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