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Lattice Boltzmann simulation of the movement of droplets on stripe-patterned surfaces having different wettability

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ABSTRACT

A stripe-patterned surface with different wettability can be effective for the passive control of droplet movement on a vertical surface. We have performed three-dimensional Lattice Boltzmann (LB) simulations to investigate the effect of the pattern characteristics and liquid properties on the droplet movement. The simulation was initiated by imposing gravity on the droplet formed on the surface. The droplet moves along the direction of the pattern when the angle between the gravity and the pattern is small; however, it starts to overrun the stripes when the angle is greater than a certain value, i.e., critical angle. It is shown that the critical angle decreases as the Bond number increases while it increases as the strength of the adhesion/repulsion force increases. The droplet forms a curved asymmetric boundary on the stripe-patterned surface due to gravity and surface forces. The critical angle is also affected by the thickness of the stripes.

1. Introduction

Control of a liquid droplet movement on a surface is an essential technology for a wide range of applications including micro-fluidic devices [1], fuel cells [2], oil recovery [3], and water gathering systems [4]. There are active and passive systems depending on whether or not it uses thermal or electrical energy to change the surface tension between the droplet and surface. Examples of active systems include a switchable thermo-sensitive surface [5], which is used as a micro-fluidic valve for a lab-on-a-chip system [6]. Lahann et al. [7] showed that the contact angle of liquid droplet changes on a switchable surface in response to an electrical potential. Using two sets of opposing planar electrodes fabricated on glass substrates, Pollack et al. [8] demonstrated positional and formational control of microdroplets by electrowetting-based actuation. Small droplets in microscale can be effectively controlled by an active system; however, it may not be a feasible technique in macro-scale due to an excessive cost to cover a large area [9]. A passive system, however, utilizes the permanent wettability gradient with no external energy input and therefore, it can only change the direction of the droplet movement. Wettability gradient can be achieved by a chemical gradient surface [10] and a textured glass structure with a wide range of curvature gradients [11]. Xu et al. showed that a water droplet can follow the S-curved line having different wettability on a declined surface [12]. Suzuki et al. showed that a water droplet can move along the direction of the stripe pattern that has different wettability [13]. Among various surface patterns, the stripe pattern has the maximum difference in wettability between the vertical and horizontal directions [14].

In a passive system utilizing the stripe pattern with different wettability, the movement of droplets is affected by gravity, liquid property, and several surface features including stripe thickness, the strength of surface force, and the slope of the pattern to gravity. Suzuki et al. showed the sliding behavior of water droplets on a stripe-patterned surface for two different wettability conditions and stripe thicknesses [13]. He observed that the droplet boundary is distorted on the patterned surface but it was difficult to determine precisely the characteristics of the droplet movement. Therefore, a three-dimensional simulation may be necessary to extensively investigate not only the details of the droplet movement on the patterned surface but also the effect of the droplet properties and pattern characteristics on the droplet movement.

Simulation of multiphase flow has been a challenging task due to the complexity of deformable and arbitrary interface between different phases. In conventional computational fluid dynamics (CFD) methods, a special treatment involving techniques such as volume of fluid (VOF) [15] and level set methods [16] is necessary to determine the characteristics of the interface at every moment. The implementation of phase separation and interaction between different phases is relatively simple in the lattice Boltzmann method (LBM) since the model can easily incorporate multiple components and set

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the interaction forces to create interface between different components. Many models have been suggested to study various interface phenomena such as the color-fluid model [17], the interparticle-potential model [18–20], the free energy model [21,22], and the mean-field theory model [23,24]. The wettability of a liquid droplet on the solid surface can be simulated by introducing interaction forces between the solid surface and the fluid. This technique has been applied to study the spreading behavior of liquid on certain substrate patterns [25,26], droplet motion on a surface with wettability gradient [27], droplet movement at the interface of different wettibilities [28], and the anisotropic wetting velocity on a stripe-patterned surface [29].

In this work, the movement of droplet on a stripe-patterned surface has been observed through three-dimensional multiphase/multicomponent LBM simulation. We have simulated the droplet movement on the vertical surface under external forces consisting of gravity and surface force. We have investigated how the movement of droplet is affected by such external forces in terms of the strength of wettability, droplet property, and several design features including stripe thickness and the slope of the pattern to gravity.

2. Lattice Boltzmann modeling

The LB model in this work is based on the multi-component multiphase interparticle potential model developed by Shan and Chen [18]. In most cases, for simplicity, it is assumed that each of the components has the same density and ideal equation of state and every two components are separated by a repulsive force. The distribution function for each component has the same relaxation time in a three-dimensional 19-speed (D3Q19) lattice, as described by the following equation:

$$f_i^k(\boldsymbol{x}+\boldsymbol{e_i}\delta_t,\ t+\delta_t) = f_i^k(\boldsymbol{x},\ t) - \frac{f_i^k(\boldsymbol{x},\ t) - f_i^{k(eq)}(\boldsymbol{x},\ t)}{\tau_k} \tag{1}$$

where f_i^k is the density distribution function, i is velocity direction, k is the number of fluid, x is position, t is time, δ_t is time increment, and τ_k is the relaxation time. $f_i^{k(eq)}(\boldsymbol{x}, t)$ is the equilibrium distribution function that is defined as:

$$f_i^{k(eq)} = w_i\rho_k\left[1 + \frac{\boldsymbol{e_i}\cdot\boldsymbol{u}_k^{eq}}{c_s^2} + \frac{1}{2}\frac{\left(\boldsymbol{e_i}\cdot\boldsymbol{u}_k^{eq}\right)^2}{c_s^2} - \frac{1}{2}\frac{\left(\boldsymbol{u}_k^{eq}\right)^2}{c_s^2}\right] \tag{2}$$

where w_i is 1/18 for $i = \{1, 2, 3, 4, 5, 6\}$, w_i is 1/36 for $i = \{7, 8, 9, \ldots, 17, 18\}$, and w_i is 1/3 for $i = \{0\}$. c_s is the speed of sound in the lattice and assumed as $1/\sqrt{3}$ in this work. The unit velocity vectors are chosen as

$$\boldsymbol{e}_i = \begin{cases} (0,0,0),\ i=0 \\ (\pm1,0,0),(0,\pm1,0),(0,0,\pm1),\ i=1\sim6 \\ (\pm1,\pm1,0),\ (\pm1,0,\pm1),(0,\pm1,\pm1), i=7\sim18 \end{cases} \tag{3}$$

The viscosity of the fluid is defined as:

$$\nu = c_s^2\left(\tau - \frac{1}{2}\right)\delta_t \tag{4}$$

The density, ρ^k, and velocity $\boldsymbol{u}_k$ at each lattice can be calculated as follows:

$$\rho_k = \sum_i f_i^k \tag{5}$$

$$\boldsymbol{u}_k = \frac{1}{\rho_k}\sum_i \boldsymbol{e_i}\cdot f_i^k \tag{6}$$

In the presence of external force, the equilibrium velocity in Eq. (2) is calculated as:

$$\rho_k\boldsymbol{u}_k^{eq} = \rho_k\boldsymbol{u}' + \tau_k\boldsymbol{F}_k \tag{7}$$

where $\boldsymbol{u}'$ is the common velocity of two components given by,

$$\boldsymbol{u}' = \frac{\left(\sum_k \frac{\rho_k\boldsymbol{u}_k}{\tau_k}\right)}{\left(\sum_k \frac{\rho_k}{\tau_k}\right)} \tag{8}$$

The total interactive force $\boldsymbol{F}_k$ consists of the fluid/fluid interactive force $\boldsymbol{F}_{1k}$, the fluid/solid interactive force $\boldsymbol{F}_{2k}$, and gravity $\boldsymbol{F}_{3k}$. $\boldsymbol{F}_{1k}$ is given as,

$$\boldsymbol{F}_{1k}(\boldsymbol{x}) = -\psi_k(\boldsymbol{x})\sum_{\bar{k}} G_{k\bar{k}}\sum_i w_i\psi_{\bar{k}}(\boldsymbol{x}+\boldsymbol{e}_i)\boldsymbol{e}_i. \tag{9}$$

where $\psi_k(\boldsymbol{x})$ is the interaction potential of the k component commonly taken as the density and $G_{k\bar{k}}$ is the interaction strength. The force imposed on the k component consists of two parts. One is the force between the same components and the other is the force between different components. The former is the attractive or repulsive force between the same components and non-zero G_{kk} results in a non-ideal value. The latter is the repulsive force between different components and causes separation of the two components. The density of each component is chosen for the $\psi_k(\boldsymbol{x})$ of two immiscible ideal fluids. The pressure of fluid is calculated as [30]:

$$p = c_s^2\rho + \frac{c_s^2}{2}\sum_{k\bar{k}} G_{k\bar{k}}\psi_k\psi_{\bar{k}}, \tag{10}$$

The force at the interface between the fluid and solid wall is given as:

$$\boldsymbol{F}_{2k}(\boldsymbol{x}) = -\psi_k(\boldsymbol{x})\sum^{G_{ks}} w_i s(\boldsymbol{x}+\boldsymbol{e}_i)\boldsymbol{e}_i \tag{11}$$

where G_{ks} is the interaction strength between the solid wall and the k component of the fluid. $s(\boldsymbol{x})$ is a function to indicate the solid wall and it is 1 on the solid wall and 0 otherwise. The contact angle between the fluid and solid is determined graphically based on simulation results for different values of $G_{k\bar{k}}$ and G_{ks}. Finally, gravity can be simply introduced as,

$$\boldsymbol{F}_{3k}(\boldsymbol{x}) = \rho_k\boldsymbol{g}, \tag{12}$$

where $\boldsymbol{g}$ is the acceleration due to gravity.

The bottom surface where the droplet is formed and the top surface that is parallel to the bottom surface were treated as solid walls using the bounce back scheme [31]. Periodic conditions were applied for other two pairs of parallel surfaces.

The lattice units (lu), time steps (ts), and mass units (mu) are the units of length, time, and mass, respectively.

3. Simulation

Fig. 1 shows the schematic diagram of the droplet on the stripe-patterned surface. An additional set of coordinates is introduced to indicate the direction of the pattern: direction 1 is the longitudinal direction of the pattern and direction 2 is normal to direction 1 on the x–y plane. The numerical domain consists of $80 \times 80 \times 40$ lattice points in the 1-, 2-, and z-direction, respectively. The simulation starts from creating a half-sphere droplet on the vertical wall. The radius, r_0, of the droplet is initially given as 25 lu. The density and viscosity are the same for the two components and component 1 represents the droplet. The density of component 1 is set as 1.0 inside the droplet and 0.01 outside the droplet. The density of component 2 is set as vice versa. The interparticle strengths are given as $G_{12} = G_{21} = 2.00$, $G_{11} = G_{22} = 0.00$ and $G_{2s} = 0.00$. G_{1s} varies for different contact angles. The boundary of the droplet is assumed to exist where the density of fluid 1 is 0.5. The droplet deforms from its original shape due to uneven surface forces at the droplet boundary. We assumed that the droplet reached its steady shape when the variance of the total weight is less than 10^{-6} % with time.

The stripe-patterned surface is characterized by the thickness of the stripe, Δs, the slope angle, α, and the interaction strengths,