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Study of transporting of droplets on heterogeneous surface structure using the lattice Boltzmann approach

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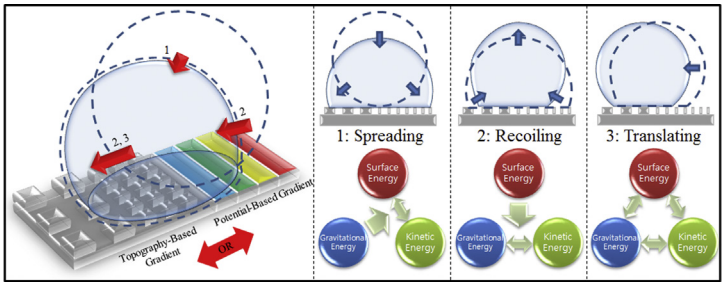
GRAPHICAL ABSTRACT



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ABSTRACT

Droplet movement on heterogeneous surfaces was simulated with a computational fluid dynamics (CFD) modeling method known as the lattice Boltzmann method (LBM). Motions of droplets were also analyzed in terms of kinetic, gravitational, and surface free energy. The first part of this study focused on the transportation of droplets by chemical actuation on a surface divided by five chemical bends, each having a different hydrophobicity, establishing a gradual progression from hydrophobic to hydrophilic phases. The second part of this study focused on the transportation of droplets by a surface with a structural gradient having its two halves textured with microscopic pillars, corresponding to a difference in hydrophobicity. In the first part of the study, the numerical results showed that a droplet tended to move to a less hydrophobic region with surface free energy reduction by spreading and decaying. This indicates that the surface free energy was converted into kinetic energy and gave mobility to the droplet. In the second part, three steps of the droplet motion were observed: spreading, recoiling, and translation.

1. Introduction

In microfluidic systems, the surface tension plays an important role in droplet motion [1]. Therefore, in these systems, manipulating surface tensions or surface energy gradients can provide a driving force for droplet transportation. Since the first investigation by Brochard [1], diverse techniques have been described for such surface manipulations: the establishment of a gradient of chemical potential [2,3] or thermal potential [4]; electrowetting on a dielectric [5]; capillary ratcheting [6]; and surface patterning [7–11]. Among these, changing the surface material and patterning the surface can cause a droplet to move in the absence of external forces. For example, Lai et al. [9] designed a surface structure with microribs and controlled wettability by changing their pitches; Sommers et al. [10] created scratched surfaces on metallic substrates by laser-

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etching; and Guo et al. [11] implemented a taper-ratchet array and applied vibration to the surface to move a droplet. These studies included the collection of experimental data on the contact angles (CAs), velocities, displacements, and net forces.

Following the above experimental studies, several groups performed theoretical analysis to solve directional driving characteristics [12,13]. For example, Fang et al. [12] derived equations to calculate the energy barrier during a change in the configuration of a micropillar array, and Bai et al. [13] obtained equations describing driving forces by considering chemical force, hysteresis resistance due to CA hysteresis, and the Laplace force induced by the curvature gradient.

Though the surface fabrication skills that are necessary to implement the above mentioned droplet transport mechanisms are already well developed, the analytical studies still lack sufficient understanding of the fundamental concept to perform an optimized and parametric study. Although the theoretical works referenced above have calculated the driving forces and the energy barrier of directional movement of a droplet, they have assumed that the interface is configured either in a state of complete wetting (the Wenzel state) or a state of composite wetting with an air pocket underneath (the Cassie state). These assumptions are somewhat unrealistic compared to shapes of actual interfaces. To predict the exact motion of droplets, it is essential to improve our knowledge of the actual interface configurations and the areas of the interfaces.

To complement the above theoretical approaches, other researchers have proposed the calculation of interface configurations through numerical approaches. Liao et al. [14] simulated liquid droplets on horizontal and inclined plates with surface energy gradients, showing the equilibrium shapes of droplets. Also, by using dynamic van der Waals theory, Xu et al. [15] simulated droplet migration on solid substrates with wettability gradients, including a detailed analysis of velocity and slip length. However, these numerical studies did not include energy analysis, which is essential for the accurate analysis of a droplet's interfacial characteristics.

Recently, using the high density ratio lattice Boltzmann model, several researchers have performed simulation works related to the behavior of a high density droplet. Lee et al. [16] simulated the dynamic behavior of an inkjet droplet impinging on a flat surface, and Liu et al. [17] simulated the deformation and breakup of a droplet or bubble in a fluid flow. As in those numerical studies, the lattice Boltzmann method (LBM) has been used as a promising numerical scheme for simulating multi-phase and multi-component fluid flows to model phase segregation and interfacial dynamics of multi-phase flows of realistic density ratio.

Accordingly, we herein simulated the transport of droplets on chemical gradients and structurally heterogeneous (gradient) surfaces using the numerical model of Yan et al. [18]. Yan's model is a kind of high density ratio lattice Boltzmann model that can control the wettability of solid surface. Furthermore, we analyzed the motions of droplets in terms of conversions among three energy states: kinetic energy, gravitational potential energy, and surface free energy. Energy analysis was used to provide a detailed interpretation of droplet motion on the gradient surface at each step.

2. Numerical method

In this section, we describe the high density ratio LBM with a partial wetting condition that we used for this research. This numerical method, proposed by Yan et al. [18], considers an incompressible two-phase flow with a high density ratio (Inamuro et al. [19]) and the wetting condition (Briant et al. [20]).

2.1. High density ratio and wetting condition in LBM

For a three-dimensional LBM model (D3Q15), the particle velocity e_i ($i = 0,1,\ldots,14$) is given by

$$[e_0,e_1,e_2,e_3,e_4,e_5,e_6,e_7,e_8,e_9,e_{10},e_{11},e_{12},e_{13},e_{14}] = \begin{bmatrix} 0 & 1 & 0 & 0 & -1 & 0 & 0 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 \\ 0 & 0 & 1 & 0 & 0 & -1 & 0 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 1 & 0 & 0 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 \end{bmatrix}. \tag{1}$$

To simulate a two-phase fluid flow, two particle velocity distribution functions are used to overcome numerical instability for interfaces with large density differences. Functions f_i and g_i are used to calculate the order of a parameter φ that distinguishes the two phases, and the predicted velocity u^* in the absence of a pressure gradient. The evolution of the particle distribution functions $f_i(x,t)$ and $g_i(x,t)$ with particle velocity e_i at point x and time t is calculated by using the following equations:

$$f_i(x + e_i\delta_t, t + \delta_t) = f_i^{eq}(x,t), \tag{2}$$

$$g_i(x + e_i\delta_t, t + \delta_t) = g_i^{eq}(x,t), \tag{3}$$

$$f_i^{eq}(x,t) = Q_i\phi + F_i\left[p_0 - k\phi\nabla^2\phi - \frac{k}{6}|\nabla\phi|^2\right] + 3\omega_i\phi(e_i'\cdot u) + \omega_i k e_i'\cdot G(\phi)\cdot e_i, \tag{4}$$

$$g_i^{eq}(x,t) = \omega_i\left[1 + 3(e_i'\cdot u) + \frac{9}{2}(e_i'\cdot u)^2 - \frac{3}{2}u^2 + \frac{3}{4}e_i'\cdot(\nabla u + u\nabla)\cdot e_i\right] + \omega_i\frac{k}{\rho}e_i'\cdot G(\phi)\cdot e_i - \frac{2}{3}F_i\frac{k}{\rho}|\nabla\phi|^2 + 3\omega_i\frac{1}{\rho}\cdot[\mu(\nabla u + u\nabla)]e_i, \tag{5}$$

where $\delta_t = 1$ is the time step during which the particle travels the lattice spacing; f_i^{eq} and g_i^{eq} are the corresponding equilibrium states of f_i and g_i; and u, ρ, and μ are the macroscopic velocity, density, and dynamic viscosity, respectively. k is a constant parameter determining the width of the interface and the strength of the surface tension. The parameters ω_i, F_i, Q_i, and $G(\varphi)$ are given as follows:

$$\omega_i = \begin{cases} 2/9, & i = 0, \\ 1/9, & i = 1,\cdots,6, \\ 1/72, & i = 7,\cdots,14, \end{cases} \tag{6}$$

$$F_i = \begin{cases} -7/3, & i = 0, \\ 1/3, & i = 1,\cdots,6, \\ 1/24, & i = 7,\cdots,14, \end{cases} \tag{7}$$

$$Q_i = \begin{cases} 1, & i = 0, \\ 0, & i = 1,\cdots,14, \end{cases} \tag{8}$$

$$G(\phi) = \frac{9}{2}(\nabla\phi)(\phi\nabla) - \frac{3}{2}|\nabla\phi|^2 I. \tag{9}$$

In the above equations, I is a unit tensor of second order. The parameter p_0 is based on the bulk free-energy density $\psi(\varphi)$ as follows:

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