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Lattice Boltzmann simulations of forced wetting transitions of drops on superhydrophobic surfaces

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ABSTRACT

The behavior of drops on superhydrophobic surfaces is of interest from an engineering point of view. As it can be difficult to probe some of the more subtle phenomena by experiment, numerical simulations can be illuminating. Many research efforts have utilized the lattice Boltzmann method to glean important conclusions about the nature of this subject, but only few have done so while eliminating the phenomenon of spurious currents and employing drop densities greater than approximately ten times that of the gas density. This paper presents a new implementation of boundary conditions for the complex geometry found in simulations of drops on superhydrophobic surfaces, which extends an existing model that has been shown to eliminate spurious currents. We validate our model by comparison with experiments, and demonstrate that spurious currents are eliminated for the density ratio encountered in a water/air system. We further discuss the issue of numerical resolution for a problem that possesses such a naturally large separation of scales, and we present a comparison between two- and three-dimensional simulations. We find that an adequate resolution, which may be difficult to achieve, must be given to capture the appropriate transition from the Cassie to the Wenzel state for the case of forced wetting under gravity. Furthermore, the form of our boundary condition may be extended to cover other types of complex geometry not included here.

1. Introduction

Drops deposited on topographically patterned surfaces can exhibit interesting behavior. The understanding of this behavior can be invaluable in areas such as ink-jet printing, microfluidic technology, and self-cleaning surface applications. A surface that is hydrophobic in nature, can become a superhydrophobic surface when it is patterned with a geometrical roughness, typically on the order of microns [1,2]. The interaction between the drop and the roughness acts to increase the inherent hydrophobicity of the substrate. Water drops on surfaces coated with low surface energy substances, though microscopically flat, typically cannot achieve a contact angle greater than 120° [3]. On a superhydrophobic surface however, a water drop can achieve contact angles up to around 170°, simply as a result of the geometrical patterning [4–6]. The roughness can be effective regardless of whether it is disordered, as in many cases in nature, or ordered, as can be achieved by micro-fabrication technology [7].

Drops can exist in one of two states on a superhydrophobic surface. The drop can be suspended on top of the roughness, without touching the underlying substrate; this is known as the Cassie state [8]. A decreased adhesion between the drop and

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the solid surface, due to the presence of gaps between the areas of contact, is responsible for interesting behavior such as the increased contact angle (*cf.* Fig. 3 in Section 3.1) and decreased drag on an inclined surface [9]. The drop can also be sunken into the roughness to contact the underlying substrate; this is known as the Wenzel state [10]. The drop also experiences an increased contact angle in this case, but the motion of a drop in this state is more restricted due to hysteresis and contact line pinning [11]. As the two states have markedly distinct behavior, one is interested in the conditions that determine the individual states. From thermodynamic theories [12,13], one can determine whether the Cassie or Wenzel states are thermodynamically stable. It is possible for both states to be stable, but typically the Wenzel state is the lower energy state. In that case, the Cassie state is meta-stable, as an energy barrier must be crossed in order to transition to the thermodynamically preferred Wenzel state. The transition to the Wenzel state is therefore irreversible in that case [14,15]. Although thermodynamic theories are useful for predicting characteristics of the final state, an understanding of the transition process is not fully known. As the process is difficult to investigate experimentally, a numerical exploration can be enlightening.

The lattice Boltzmann method (LBM) is a powerful tool for simulating Navier–Stokes fluid behavior [16]. Our particular scheme models multi-phase flows by including intermolecular forces at a mesoscopic level to recover surface tension effects at interfaces at a macroscopic level [17–24]. The intermolecular forces are derived by minimizing the free energy in the system, where a diffuse interface approach is used to model the interface [25]; an extensive discussion of diffuse interfaces in the LBM was given by Kang et al. [26]. The interaction between the interface and the solid surface is captured by incorporating a wall free energy into the expression of the total free energy [27].

Dupuis and Yeomans [28] were the first to use the LBM to model drops on a superhydrophobic surface. The LBM was subsequently used to study Cassie-Wenzel transition [29–31], contact angle hysteresis [32], drop morphology [33,34], drop impact [35], and drop motion on superhydrophobic surfaces [36–38]. A significant issue with many of these methods is that they cannot eliminate the unwanted phenomenon of *spurious currents*. Spurious currents are unphysical fluid motions, caused by an inaccurate discretization of the surface tension term, which do not fade with time [39]. As spurious currents are exacerbated by large density ratios and the presence of walls, many of these works were limited to employing drop densities no greater than approximately ten times that of the gas density, though some were able to eliminate the currents and use large density ratios [36,34,37].

We present an extension of the method of Lee and Liu [24] to implement boundary conditions for the complex geometry of superhydrophobic surfaces, in particular for the sharp edges and corners of the pillars. Our boundary conditions eliminate the spurious currents at equilibrium, and allow us to simulate the density ratio of a water–air system. Our simulations also conserve mass approximately; a change of mass no greater than 1% is observed. We use these boundary conditions to simulate forced wetting under gravity of a drop on a superhydrophobic surface. We compare our results with the experimental results of Barbieri et al. [40]. We find that our simulations reproduce the experimental contact angles well, both in the Cassie and in the Wenzel state, but the transition to the Wenzel state is predicted prematurely compared to the experiments.

The rest of the paper is summarized as follows. In Section 2 we detail our numerical method, including the new boundary conditions in Section 2.3. We present our model validation in Section 3, along with a proof of the elimination of spurious currents in Section 3.2, and some comparisons between two- and three-dimensional simulations in Section 3.3. We discuss some conclusions in Section 4.

2. Numerical method

The numerical implementation used is that of Lee and Liu [24]. The innovation of this paper is primarily contained in the handling of the complex boundaries. The Cahn–Hilliard, pressure evolution, and momentum equations are recovered from our lattice Boltzmann equations which govern the evolution of the physical system. The distribution function for mass and momentum is transformed into the distribution function for pressure evolution and momentum, while a supplemental distribution function for the composition is introduced. The lattice Boltzmann equations are obtained by applying the trapezoid rule along characteristics to the discrete Boltzmann equations. Zero-flux conditions are applied at solid boundaries to prevent unphysical mass and momentum transfer through the boundary nodes.

2.1. Cahn–Hilliard model

The Cahn–Hilliard model [41] for a binary system of incompressible, immiscible fluids describes the evolution of the composition, C, of the system as it progresses towards its equilibrium state. The volume fraction of component 1, the heavier fluid say, is C, and the local densities of the species are $\tilde{\rho}_1 = C\rho_1$ and $\tilde{\rho}_2 = (1-C)\rho_2$ [42]. The mixture density, $\rho = \tilde{\rho}_1 + \tilde{\rho}_2 = C\rho_1 + (1-C)\rho_2$, is a linear function of the composition. The continuity equation for species i is written:

$$\frac{\partial \tilde{\rho}_i}{\partial t} + \nabla \cdot \tilde{\rho}_i \boldsymbol{u}_i = 0, \quad i = 1, 2. \tag{1}$$

Here $\boldsymbol{u}_i$ is the local velocity of species i and is related to the volume averaged velocity $\boldsymbol{u}$ by $\rho_i \boldsymbol{j}_i = \tilde{\rho}_i(\boldsymbol{u}_i - \boldsymbol{u})$, where $\boldsymbol{j}_i$ is the volume diffusive flow rate of species i. Furthermore, if the diffusive flow rate is related to the composition, $\boldsymbol{j}_1 = -\boldsymbol{j}_2 = \boldsymbol{j}$, which leads to $\nabla \cdot \boldsymbol{u} = 0$ [42]. Finally, the convective Cahn–Hilliard equation is given by rewriting Eq. (1) as