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A lattice Boltzmann model for substrates with regularly structured surface roughness

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ABSTRACT

Superhydrophobic surface characteristics are important in many industrial applications, ranging from the textile to the military. It was observed that surfaces fabricated with nano/micro roughness can manipulate the droplet contact angle, thus providing an opportunity to control the droplet wetting characteristics. The Shan and Chen (SC) lattice Boltzmann model (LBM) is a good numerical tool, which holds strong potentials to qualify for simulating droplets wettability. This is due to its realistic nature of droplet contact angle (CA) prediction on flat smooth surfaces. But SC-LBM was not able to replicate the CA on rough surfaces because it lacks a real representation of the physics at work under these conditions. By using a correction factor to influence the interfacial tension within the asperities, the physical forces acting on the droplet at its contact lines were mimicked. This approach allowed the model to replicate some experimentally confirmed Wenzel and Cassie wetting cases. Regular roughness structures with different spacing were used to validate the study using the classical Wenzel and Cassie equations. The present work highlights the strength and weakness of the SC model and attempts to qualitatively conform it to the fundamental physics, which causes a change in the droplet apparent contact angle, when placed on nano/micro structured surfaces.

1. Introduction

The contact angle measures the ability of a liquid to spread on a surface. When a droplet is deposited on a planar solid surface, the contact angle can be defined as the angle at which the outline tangent of a liquid drop meets a solid surface. Depending on the value of the contact angle, surface properties are determined as hydrophobic ($\theta > 90$ degrees) or hydrophilic ($\theta < 90$ degrees). Superhydrophobic surfaces are surfaces with contact angles greater than 150 degrees.

The contact angle is determined from the condition of minimizing the total energy of the system $dE_{Tot} = 0$, which leads to Young's equation. Young's equation determines the static contact angle through balancing the surface and interfacial tensions $\gamma_{\sigma\sigma'}$ (σ, σ' inidicate solid–liquid, solid–air and liquid–air) shown in Fig. 1. Young's equation is a clear simplification of the real physics of droplet spreading and it is valid only for smooth homogeneous surfaces.

For rough surfaces, which are commonly used for creating superhydrophobic substrates, Wenzel [1] and Cassie–Baxter [2] suggested modified versions of Young's equation for calculating the apparent contact angle.

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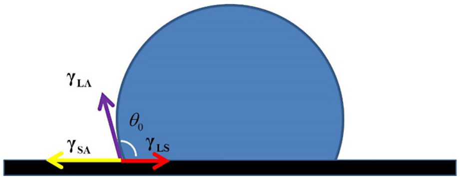

Fig. 1. Description of the forces per unit length acting on the contact line of a liquid droplet deposited on a flat smooth surface at equilibrium.

Superhydrophobic surfaces are in high demand, because properties such as anti-sticking, anti-contamination and self-cleaning are useful. Superhydrophobic surfaces are desired in many industrial applications such as, self-cleaning windshields for vehicles, the separation of water and oil, drug delivery, and the manufacture of water-proof and fire repellant clothing. Increasing the surface roughness for low surface energy materials is the main approach that has been developed to generate superhydrophobic surfaces, and the contact angle is the main method to characterize the surface super-hydrophobicity.

Numerous scientific papers have demonstrated how important roughness is for superhydrophobic surfaces and have focused on the relation between contact angles and surface geometry [3–5]. It was of particular interest to understand which regime describes most accurately the phenomenon of liquid wetting of structured surfaces. In [6–8] water wettability was investigated experimentally on surfaces comprising of pillars with different aspect ratios. By varying the aspect ratio R (width of the pillars to the spacing between the pillars) it was shown that at low aspect ratios the wettability was described by the Wenzel model. Increasing R led to a change from the Wenzel to Cassie wettability states. Other studies [9–12] provided theoretical hypothesis for understanding wettability on rough surfaces by using an array of square pillars. These studies evaluated the wettability by using the Wenzel and Cassie models, and established the conditions for the existence of the Wenzel and Cassie regimes. The wettability in the Wenzel and Cassie regimes was studied in detail in Refs. [13–16]. It was shown, that there is a critical value of the aspect ratio R above which the Wenzel regime is thermodynamically more stable and below which the Cassie regime exists. Quéré [17] showed that metastable Cassie drops may form on surfaces, which thermodynamically prefer the Wenzel regime. The metastability was demonstrated in several ways, and that the state of the droplet depended on the amount of liquid as well as the means of depositing the liquid on the surface.

In order to understand the relation between the wettability of a surface and droplet spreading mechanism, various numerical models were developed. The numerical schemes involved in these models included continuum approach based models such as VOF studies used by Trapaga and coworkers [18,19], Lagrangian finite-element methods used by Fukai et al. [20,21], level-set approach developed by Zheng and Zhang [22], and lattice-Boltzmann models (LBM) such as free energy approach used by Dupuis and Yeomans [23], large density based Inamuro model used by Yan and Zu [24] and Yong et al. [25], two color model used by Rothman and coworkers [26] and Halliday and coworkers [27] and the pseudo-potential based approach developed by Shan and Chen [28]. Though the sharp interface developed by the continuum approach based models has an advantage over diffuse interface based lattice Boltzmann models, the interface modeling and complex grid adaptability of continuum models made it difficult to handle the problems related to droplet wetting and droplet dynamics. The inherent interface forming mechanism of LBM along with the nonlocal interaction potential among the nearest-neighboring particles made the pseudo-potential LBM [28] a good numerical tool for simulating multi-phase and multi-component flows. The scheme was first proposed by Shan and Chen, and thus will be further referred to as Shan and Chen (SC) model in the present manuscript.

Martys and Chen [29] improved the SC model further by projecting the original scheme from 4D FCHC into D3Q19 regular lattice, and added gravity and fluid–solid interaction forces to simulate multi-component flows in porous media. This LBM model has been used in the study of fluid–solid interaction in microchannels, on flat and rough surfaces. Raiskinmäki et al. [30] simulated spreading of small droplets on smooth and rough solid surfaces using the three-dimensional LBM and found that this method can indeed be very useful in such studies. Schmieschek and Harting [31] studied the dependence of the contact angle on some geometrical measurements and model parameters such as the curvature, system size, initial droplet volume, coupling parameter and wetting parameter (pseudo density). They showed that the dependence of contact angle on the model parameters is stronger than its dependence on the geometric measurements. The effect of surface topography on the contact angle hysteresis has been studied by Hyväluoma [32]. By using LBM-SC multiphase model, they simulated droplets sliding on an anisotropic surface. The study showed that the contact angle hysteresis decreased as the surface becomes more hydrophobic. Hyväluoma concluded that the contact angle hysteresis is a better parameter for the purpose of characterizing the super-hydrophobicity. Sbragaglia et al. [33] presented a multiphase flows LBM to describe the wetting and de-wetting transition of fluids in the presence of complex geometries in micro and nano-devices. The study concluded that the physics of the boundary conditions is quantitatively reproduced by modeling the fluid at mesoscopic level, and showed the possibility to design smart surfaces by combining geometry and hydrophobicity, with slippage properties that can be changed by a control parameter.

Previous studies indicate that the SC model can be used for wide range of wetting studies in order to understand the effect of curved surfaces, droplet volume, surface wetting characteristics, wetting and de-wetting transitions and surfaces with different wetting characteristics. However, most of these studies involved flat surfaces or rough surfaces [25,32], which geometrical parameters (pillar size to droplet radius) did not warrant a realistic representation of the wetting state presented