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Roughness Effects on Continuous and Discrete Flows in Superhydrophobic Microchannels

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Abstract. The dynamic behaviors of continuous and discrete flows in superhydrophobic microchannels are investigated with a lattice Boltzmann model. Typical characters of the superhydrophobic phenomenon are well observed from our simulations, including air trapped in the surface microstructures, high contact angles, low contact angle hysteresis, and reduced friction to fluid motions. Increasing the roughness of a hydrophobic surface can produce a large flow rate through the channel due to the trapped air, implying less friction or large apparent slip. The apparent slip length appears to be independent to the channel width and could be considered as a surface property. For a moving droplet, its behavior is affected by the surface roughness from two aspects: the contact angle difference between its two ends and the surface-liquid interfacial friction. As a consequence, the resulting droplet velocity changes with the surface roughness as firstly decreasing and then increasing. Simulation results are also compared with experimental observations and better agreement has been obtained than that from other numerical method. The information from this study could be valuable for microfluidic systems.

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Key words: Lattice Boltzmann method, interfacial slip, superhydrophobicity, solid-fluid interaction, roughness effect, microchannels.

1 Introduction

Superhydrophobic surfaces have recently been studied extensively for both scientific and engineering interests [10,20,21,37]. Most of these studies focus mainly on the contact angle behaviors. Due to the air trapped between the microstructures, the adhesion between

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the surface and liquid is reduced and a droplet on such a surface exhibits high contact angles and low contact angle hysteresis (the difference between the advancing and receding angles). On the other side, Kim et al. [15] examined the sliding angles of droplets on rough hydrophobic surfaces and found that the friction from the solid surfaces to the liquid was greatly reduced. Richard and Quere [25] had also studied the drop moving behaviors on inclined surfaces. The drop was observed rolling down the superhydrophobic surface instead of sliding on hydrophilic surfaces. Takeda et al. [32] conducted other interesting experiments showing that a vertical electric field can lift a water droplet to jump up from a superhydrophobic surface.

Recently, several experiments have shown that the surface friction to continuous flows can also be reduced by employing superhydrophobic surfaces [5, 6, 9, 14, 18, 22]. These works demonstrated that the adhesion and friction between the liquid and superhydrophobic surfaces have been greatly reduced. However, contradictory to these experiments, theoretical and numerical investigations of this interesting and promising phenomenon are rare due to the difficulties from the geometric complexity, fluid dynamics, interfacial rheology, and multiple phases (liquid, vapor, and solid) involved; especially for discrete flows in spite of their attractiveness in digital microfluidics [8, 12].

Studying on fluid slip over a solid surface has long been an interesting subject since the pioneering work by Navier and Maxwell [41]. Recent measurements indeed indicate significant slip on solid surfaces [4,33,45]. Due to the difficulties in direct microscopic observation near the solid-fluid interface, numerical simulations, by means of molecular dynamics (MD) [7] and the lattice Boltzmann method (LBM) [27,41], have been employed to study the underlying mechanism and relationship between fluid slip and the properties of fluid and solid. In general, both experimental and simulation results show that there is a strong relationship between the magnitude of slip and the solid-fluid interaction: the weaker the interaction, the larger the contact angle and hence the slip. These studies are also usually conducted on smooth surfaces or continuous flows, and the roughness effects on continuous and discrete flow behaviors have not been well examined. Therefore, it is interesting and important to investigate the superhydrophobic effects on the fluid behaviors. A better understanding of the underlying physics will also provide guidance for the design and applications of superhydrophobic materials. In this paper, we present our LBM numerical studies on the continuous and discrete flow behaviors in rough and hydrophobic channels.

2 The mean-field free energy multiphase LBM model

Our simulations employ a recently proposed mean-field free energy LBM model for non-ideal fluids for its physical representation of the solid-fluid interactions [44]. According to the mean-field version of the van der Waals theory, the total free energy F for a fluid system can be expressed as [26, 30, 40]

$$F=\int d\mathbf{r}\Big\{\psi[\rho(\mathbf{r})]+\frac{1}{2}\rho(\mathbf{r})\int d\mathbf{r}'\phi_{ff}(\mathbf{r}'-\mathbf{r})[\rho(\mathbf{r}')-\rho(\mathbf{r})]+\rho(\mathbf{r})V(\mathbf{r})\Big\}, \tag{2.1}$$