Lattice Boltzmann Study of Bubbles on a Patterned Superhydrophobic Surface under Shear Flow

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Abstract. This paper studies shear flow over a 2D patterned superhydrophobic surface using lattice Boltzmann method (LBM). Single component Shan-Chen multiphase model and Carnahan-Starling EOS are adopted to handle the liquid-gas flow on superhydrophobic surface with entrapped micro-bubbles. The shape of bubble interface and its influence on slip length under different shear rates are investigated. With increasing shear rate, the bubble interface deforms. Then the contact lines are depinned from the slot edges and move downstream. When the shear rate is high enough, a continuous gas layer forms. If the protrusion angle is small, the gas layer forms and collapse periodically, and accordingly the slip length changes periodically. While if the protrusion angle is large, the gas layer is steady and separates the solid wall from liquid, resulting in a very large slip length.

1. Introduction

The main differences between a hydrophobic surface and a superhydrophobic surface are surface chemistry and microstructure. And the later one is more important. Experiments illustrate that a smooth hydrophobic surface is likely to have much smaller slip length than a microstructured hydrophobic surface [1]. The mechanism is that for microstructured hydrophobic surfaces, small gas bubbles can be trapped within the grooves or holes on the surface [2], producing two different interfaces, water-solid interface and air-water interface, and the latter significantly reduces the shear stress. This is the so-called Cassie state. Joseph [3] has found that in Cassie state microns-lengths slip exhibits on superhydrophobic surfaces, while in Wenzel state there are no slips because of the larger solid-water friction with the absence of trapped air.

Much research has been done on the slip length of patterned superhydrophobic surface. Lauga [4], Zhou [5] and Ng [6] studied slip length of superhydrophobic surface analytically. They assumed the superhydrophobic surface to be hybrid no-slip and free-slip boundaries, thus the deformation of the bubble interface is neglected. However, it has been proven that shape of the air-water interface can influence the slip length dramatically (Sbragaglia [7]). Hyväluom [8] studied shear flow over an entrapped bubble using lattice Boltzmann method. They found that when the shear rate increases, slip length decreases because of the bubble deformation. However, in their study the density ratio of the multi-phase model was too small, and the contact lines were pinned to the slot edges. Their result conflicts with the results of Choi [9] and Gao [10] which found slip length increases when shear rate increases.

This paper studies shear flow over a patterned superhydrophobic surface using lattice Boltzmann method (LBM). Single component Shan-Chen multiphase model and Carnahan-Starling EOS are
adopted to handle the liquid-gas flow on superhydrophobic surface with entrapped micro-bubbles. The shape of bubble interface and its influence on slip length under different shear rates are investigated.

2. Numerical Model

2.1. Lattice Boltzmann Method

In this paper, lattice Boltzmann method is chosen to study boundary slip. The evolution equation of lattice Boltzmann method can be expressed as:

$$ f_i(x + c_i \Delta t, t + \Delta t) - f_i(x, t) = -\frac{1}{\tau} [f_i(x, t) - f_i^{(eq)}(x, t)] $$

(1)

where $f_i(x, t)$ is the particle distribution function with velocity $c_i$ at position $x$ and time $t$, $i$ is the lattice direction. $\tau$ is the relaxation time, and $f_i^{(eq)}(x, t)$ is the equilibrium distribution function given by

$$ f_i^{(eq)}(x, t) = \omega_i \rho [1 + \frac{c_i \cdot u}{c_s^2} + \frac{(c_i \cdot u)^2}{2c_s^4} - \frac{u^2}{2c_s^4}] $$

(2)

where $\omega_i$ are the weighting coefficients, and $c_i$ is the lattice sound speed. For the D2Q9 model we choose, $c_1 = 1/\sqrt{3}$, and $\omega_i$ are given by $\omega_0 = 4/9$ for $i=0$, $\omega_i = 1/9$ for $i=1\sim4$ and $\omega_i = 1/36$ for $i=5\sim8$. The macroscopic density is $\rho = \sum f_i$, and macroscopic velocity is $\rho \mathbf{u} = \sum f_i c_i$.

We use a single-component multiphase LBE model proposed by Shan and Chen [11, 12] to solve the liquid-gas flow on superhydrophobic surface. The interaction force which segregates different phases is given by

$$ F_m(x) = -\psi(x) \sum G(x, x') \psi(x')(x' - x) $$

(3)

where $G(x, x')$ is Green’s function which reflects the intensity of the interparticle interaction. For nearest-neighbor interparticle force, $G(x, x')$ can be expressed in the form

$$ G(x, x') = \begin{cases} 
  g_1 |x - x'| = 1 \\
  g_2 |x - x'| = \sqrt{2} \\
  0 & \text{otherwise}
\end{cases} $$

(4)

where $g_1 = 2g$, $g_2 = g/2$ for D2Q9 scheme.

$\psi(x)$ is the effective mass which is defined as a function of $x$ through its dependency on the local density, $\psi(x) = \rho / \rho(x)$. The equation of state (EOS) of the multiphase system is given by

$$ p = c_s^2 \rho + \frac{c_n}{2} \psi^2 $$

(5)

where $c_n = 6$ for D2Q9 scheme.

For Shan-Chen EOS, the effective mass is $\psi(\rho) = \rho_0 [1 - \exp (-\rho / \rho_0)]$. Therefore the EOS is $p = c_s^2 \rho + 0.5c_6 \rho_0^2 [1 - \exp (-\rho / \rho_0)]^2$. However, the max density ratio of Shan-Chen EOS is 58.497 which is too small for the liquid-gas flow on superhydrophobic surfaces. So we use the Carnahan-Starling (C-S) EOS [13] instead, whose max density ratio is more than 1000. The C-S EOS can be expressed as:

$$ p = \rho RT \frac{1 + b \rho / 4 + (b \rho / 4)^2 - (b \rho / 4)^3}{(1 - b \rho / 4)^3} - a \rho^2 $$

(6)

where $a = 0.4963 RT^2 T_c^2 / P_c$, $b = 0.18727 RT / P_c$. The subscript ‘c’ denotes the critical properties. $T_c = 0.3775a / bR$, $\rho_c = 0.5218 / b$. We set $a = 1$, $b = 4$, and $R = 1$ in our simulations according to Li [14].

The interaction force is incorporated into the model by the exact difference method which can be expressed in the form
\[ \Delta f_i(x,t) = f_i^{(eq)}(\rho(x,t),u+\Delta u) - f_i^{(eq)}(\rho(x,t),u) \]  \hspace{1cm} (7)

where \( \Delta u = F_{\text{int}} \delta t / \rho \). Compared to the velocity shifting method proposed by Shan and Chen, this method has better accuracy.

However, Gong [15] found that simulation results of Eq. 3 deviate from those obtained by Maxwell construction, especially on the vapor branch and at low temperatures. So we use a modified scheme proposed by Gong [15] which has better accuracy:

\[ F_{\text{int}}(x) = -\beta \psi(x) \sum x G(x,x') \psi(x')(x'-x) - \frac{1}{2} \beta \sum x G(x,x') \psi^2(x')(x'-x) \]  \hspace{1cm} (8)

where \( \beta \) is the weighting factor depending on the particular EOS. Gong [15] did not give the value of \( \beta \) for C-S EOS. After several simulations, we find that \( \beta = 1.22 \) for C-S EOS.

To validate the two phase model, tests of a liquid droplet in vapor are calculated. A 100×100 lattice is adopted. The initial density at the central domain with radius \( r = 30 \) is set a little higher than the critical density \( \rho_c \), and lower than \( \rho_c \) elsewhere. The periodic boundary conditions are applied in all directions. Each computation is carried out for 30000 time steps. At the steady state, a liquid droplet is formed in the central domain. Densities of liquid and gas of simulation results are compared with those of Maxwell construction, as shown in figure 1.

![Figure 1](image)

**Figure 1.** Densities of liquid phase and gas phase for C-S EOS. Our simulation result (○) is compared with analytical result (solid line)
Figure 2. Contact angle $\beta$ as a function of $\rho_w$. Our simulation result (Δ) is compared with the analytical estimate of Benzi [16] (solid line).

The fluid-solid interaction is involved by changing the wall density $\rho_w$. Here the solid wall is perceived as carrying a fictitious density $\rho_w$. Note this fictitious density is not the realistic density of the material of the solid wall. For a liquid-vapor system with densities of liquid and vapor as $\rho_l$ and $\rho_g$, respectively, setting $\rho_w=\rho_l$ leads to the contact angle $\beta=0$ and setting $\rho_w=\rho_g$ leads to $\beta=180^\circ$. To validate this method, an semicircular static droplet is initially put on a flat wall and $\rho_w$ changes. Contact angle $\beta$ as a function of $\rho_w$ is obtained, as shown in figure 2. Our numerical result coincides with analytical result [16] well when $\beta>90^\circ$.

2.2. Problem Description

We study two-dimensional Couette flow over a surface with transverse slots, as shown in figure 3. The domain is periodic in the horizontal direction. The distance between the upper and lower wall is $H$. $L_x$ and $h$ are the width and depth of the slots. $\theta$ is the protrusion angle of the gas bubble in the slot. The flow is driven by the upper wall moving with a constant speed $U_0$.

The effective slip length can be calculated from the shear stress acting on the upper wall. Because no-slip boundary condition is imposed on the upper wall, the shear stress can be calculated as $\sigma=\mu du/\partial y$. Thus the effective slip length is $b=\mu U_0/\sigma-H$, $\mu$ is the dynamic viscosity of the liquid.

In our simulations, $h=45, L=90, L_x=180, H=60$, while $U_0$ and $\theta$ change in different cases. $\tau=1.0, g=-1.0. \rho_w=0.6\rho_c$, thus the contact angle $\beta=120^\circ$. The temperature is $T=0.5T_c$, thus the densities of the liquid phase and gas phase are $3.495\rho_c$ and $0.00460\rho_c$, respectively, and the density ratio is about 760. The actual channel height is 60μm, the actual slot width is 90μm, and the actual kinetic viscosity of the fluid is $1.0\times10^{-6}$. The channel height is small in order to achieve high shear rate. Note that the kinetic viscosities of liquid and gas are the same in our simulations because of the limitation of single-component multiphase flow model. The influence of kinetic viscosity ratio is not discussed in this paper.
Figure 3. Schematic of the Couette flow over a surface with transverse slots

Figure 4. The slip length $b$ as a function of $U_0$ at $\rho_w=0.6\rho_c$ and $\theta_0=50^\circ$

Periodic boundary condition is applied in horizontal direction. Half-way bounce back boundary condition is applied to the upper wall and lower wall. Particularly, on the upper wall which is moving with speed $U_0$, the boundary condition is

$$f_i (x_j, t + \Delta t) = f_i' (x_j, t) - 2\alpha \rho \frac{c_i U_w}{c_s}$$

where $i_2$ is the opposite direction of $i$, $u_w=(U_0,0)$.

3. Results and Discussions

Figure 4 plots the slip length $b$ as a function of $U_0$ at $\theta_0=50^\circ$. The y-axis is nondimensionalized by $L$. We can see that with increasing $U_0$, the system traverses the three flow regimes in turn. In regime 1 (roughly $U_0<0.07$), the slip length is small and decreases as $U_0$ increases. In this regime, the shear rate is relatively low, the interface of the bubble deforms slightly and the contact lines are pinned to the edges of the slot, as shown in figure 5. We can see that when $U_0=0.02$, the interface is almost symmetrical. While when $U_0=0.05$, the interface deforms more obviously, and the right side (downstream) of the bubble becomes blunt thus the resistance increases and the slip length decreases.
When \(0.07 < U_0 < 0.081\), the system comes into regime 2. In this regime, the contact line on the right side of the bubble is depinned from the edge of the slot and moves downstream (see figure 5, \(U_0=0.08\)). The area of solid-liquid interface becomes smaller, thus the resistance decreases and the slip length increases.

![Figure 5. Interfaces of the bubble when \(U_0=0.02\) (solid line), 0.05 (dashed line) and 0.08 (dash dot line) respectively.](image)

If the \(U_0\) grows large enough, the depinned contact line may reach the downstream bubble, then regime 2 transits into regime 3. Unlike regime 1 and 2, regime 3 is unsteady and the interface changes periodically. At first, the downstream contact line advances and reaches the downstream bubble (figure 6(a)). Then the two contact lines coalesce and a continuous gas layer forms temporarily (figure 6(b)). However, the interface is too close to the slot edge, thus the gas layer is unstable and breaks up at the downstream slot edge (figure 6(c)). After that, the gas meniscus on top of the ridge moves rapidly downstream, driven by shear forces, and merges into the downstream slot (figure 6(d), (e)). This process then starts anew and produces a time-periodic behavior (figure 6(f)).

![Figure 6. Snapshots of the interface for \(U_0=0.082\) and \(\theta_0=50^\circ\).](image)

In figure 4, the slip length of regime 3 is averaged over one period. We can see a steep increase between regime 2 and 3. Figure 7 shows the instantaneous slip length in regime 3. The slip length varies periodically. The sharp peaks denotes the state when a continuous gas layer forms and this state coincides with Figure 6(b). Figure 7 also shows time histories of \(b\) for \(U_0=0.083\) and \(U_0=0.084\). It can be found that the period decreases as \(U_0\) increases.
Figure 7. Time history of $b$ for $U_0=0.082$ (solid line), $U_0=0.083$ (dashed line) and $U_0=0.084$ (dash dot line).

Figure 8. The slip length $b$ as a function of $U_0$ at $\rho_w=0.6\rho_c$ and $\theta_0=60^\circ$.

In the above discussion, $\theta_0$ is fixed to $50^\circ$. To study the influence of $\theta_0$, cases of $\theta_0=60^\circ$ is calculated. The slip length $b$ as a function of $U_0$ is shown in Figure 8. There are also three regimes. And regime 1 and 2 are similar to Figure 4. However, regime 3 is different. The slip length is much larger and is almost constant. The instantaneous interface is shown in Figure 9. We can see the coalescence of contact lines in Figure 9(a) and (b). But unlike Figure 6, the continuous gas layer will remains stable, as shown in Figure 9(c). The reason may be that the air layer is thicker and the interface is farer from the slot edge.

Figure 9. Snapshots of the interface for $U_0=0.07$ and $\theta_0=60^\circ$. 
4. Conclusions
This paper studies shear flow over a 2D patterned superhydrophobic surface. The shape of bubble interface and its influence on slip length under high shear rates are investigated. Following conclusions can be made:

1. A multi-phase lattice Boltzmann method is set up. Single component Shan-Chen multiphase model and Carnahan-Starling EOS are adopted. This model can well handle the large density ratio liquid-gas flow as well as the moving contact line on superhydrophobic surface with entrapped micro-bubbles.

2. At low shear rate, the interface of the bubble deforms slightly, and the slip length slightly decreases as shear rate increases because the downstream side of the bubble becomes blunt. At medium shear rate, one contact line of the bubble is depinned from the edge of the slot and moves downstream. The area of solid-liquid interface becomes smaller, and the slip length increases as shear rate increases.

3. When the shear rate is high enough, a continuous gas layer forms. The gas layer will either be steady or unsteady, depending on the protrusion angle $\theta_0$. If $\theta_0$ is small, the gas layer forms and collapse periodically, and accordingly the slip length will changes periodically. If $\theta_0$ is large, the gas layer is steady and separates the solid wall from liquid, resulting in a very large slip length.

Note that the discussions in this paper focus on 2D patterned surface. 3D multi-phase flow simulations are to be performed in order to investigate the interface phenomenon and slip length of a realistic superhydrophobic surface with 3D microstructures.

5. References
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