A lattice Boltzmann simulation of coalescence-induced droplet jumping on superhydrophobic surfaces

Fengru Ling, Gang Huang, Hao Tang, Mengmeng Geng, Yutong Ye and Zhangrong Qin*

Guangxi Collaborative Innovation Center of Multi-source Information Integration and Intelligent Processing, Guangxi Normal University, Guilin, China

*Corresponding author e-mail: qinzhangrong@gxnu.edu.cn

Abstract. The coalescence-induced droplet jumping on superhydrophobic surfaces (SHSs) observed in nature plays a significant role in energy and environmental applications. By using a three-dimensional chemical-potential-based multiphase lattice Boltzmann model, the coalescence-induced jumping of two droplets and multidroplet are systematically simulated and analysed. The results show that the size and the number of droplets and the characteristics of pillared SHSs have a strong influence on the droplet behaviour. The coalesced droplet could only jump under appropriate droplet size and characteristic parameters of SHSs. Furthermore, coalesced droplets are more likely to jump and jump higher on SHSs with larger contact angle and pillar height and smaller distance between two pillars. This work will contribute to understand the phenomenon of the coalescence-induced droplet jumping and provide theoretical guidelines for the design of new SHSs.

1. Introduction
In the past few years, increased attention has been paid to coalescence-induced droplet jumping on a superhydrophobic surface (SHS) due to its potential application in engineering fields, such as self-cleaning surfaces, condensation heat transfer performance, anti-icing and defrosting[1]. Studying the conditions under which the coalesced droplet can jump has theoretical and practical value, which deepen understanding in the phenomenon of the coalescence-induced droplet jumping and help to study new SHSs.

To clear the jumping mechanism of the coalesced droplet, intensive efforts have been devoted to conducting experiments and building models. Boreyko and Chen [2] firstly reported continuous dropwise condensation spontaneously occurring on a SHS without any external forces. They developed an inertial-capillary scaling model and found that a self-propelled jumping motion of condensate drops can be attributed to the surface energy released by drop coalescence. Liu et al. [3] adopted a two-dimensional multiphase relaxation time pseudopotential multiphase lattice Boltzmann method to simulate droplets coalescence and jumping processes on SHSs. The results revealed that coalesced droplet can jump only on a SHS with a high contact angle. In addition, Farokhirad et al. [4] reported that the coalesced droplet will not jump away from a pillared substrate if the contact angle is smaller than 120°. Moreover, the research progress has been also made on droplet jumping induced by multidroplet coalescence. Lv et al. [5] developed a general theoretical model. They found that multidroplet coalescing...
and jumping is in the majority, and the probability of three and four droplets coalescing and jumping have the highest value.

Although a lot of researchers have numerically investigated the coalescence-induced droplet jumping on SHSs, most of them only simulated the unitary case of coalescence-induced droplet jumping. Herein, the influence of different conditions, including the pillared SHS (pillar height and distance between the pillars), the contact angle, number and size of droplets, on the coalescence-induced droplet jumping is studied in details. Unlike previous studies, which mainly used the pseudo-potential model and the free energy model, we used a recently developed chemical-potential-based multiphase lattice Boltzmann model proposed by our research group [6]. This model not only satisfies Galilean invariance and thermodynamics, but calculates the contact angle simply and efficiently [7]. Due to the advantages of chemical-potential-based multiphase lattice Boltzmann model in characterizing the wettability of solid surfaces, the model can be expected to obtain more interesting results.

2. Three-dimensional chemical-potential lattice Boltzmann model

Owing to simple form, low computational cost and mature theory, the single-relaxation-time lattice Boltzmann method has become the most popular one. The evolution equation of the D3Q19 lattice Boltzmann model with single-relaxation-time collision operator can be written in a concise form as

$$\dot{f}_i(x + e_i \delta t, t + \delta t) - f_i(x, t) = -\frac{1}{\tau} \left[ f_i(x, t) - f_i^{(eq)}(\rho, u) \right],$$

(1)

where $f_i(x, t)$ is the particle distribution function at lattice site $x$, and time $t$, $e_i$ with $i = 0, \ldots, 18$ is the discrete speed, $\tau$ is the single relaxation time, $f_i^{(eq)}$ is the equilibrium density distribution function,

$$f_i^{(eq)}(\rho, u) = \rho \omega_i \left[ 1 + 3(e_i \cdot u) + 4.5(e_i \cdot u)^2 - 1.5u^2 \right],$$

(2)

where $\rho = \sum_i f_i$ and $u = \sum e_i f_i / \rho$ represent the fluid density and velocity, respectively, $\omega_i$ is the weight coefficient that are given as follows: $\omega_0 = 1/3$, $\omega_{6, 8} = 1/18$ and $\omega_{14, 18} = 1/36$.

The evolution of the lattice Boltzmann equation can be decomposed into two essential steps, namely collision and streaming. Hence, the corresponding computations of Eq. (1) can be performed as:

Collision : $\tilde{f}_i(x, t) = f_i(x, t) - \frac{1}{\tau} \left[ f_i(x, t) - f_i^{(eq)}(\rho, u) \right]$,  

(3)

Streaming : $f_i(x + e_i \delta t, t + \delta t) = \tilde{f}_i(x, t)$,

(4)

Where $f_i$ and $\tilde{f}_i$ denote pre-collision and post-collision states of the particle distribution functions, respectively.

In the process of the simulated coalescence-induced droplet jumping, the force acting on the fluid $F$ consists of $F_f$, $F_s$ and $F_b$,

$$F = F_f + F_s + F_b,$$

(5)

where $F_f$ is the fluid–fluid force[6],

$$F_f = -\rho \nabla \mu + \nabla \cdot \mathbf{P}_b(x),$$

(6)
where $\tilde{P}_0 = c_s^2 \rho \tilde{\phi}$ is the ideal-gas equation of state (EOS), $\mu$ is the chemical potential and $\rho$ is the macroscopic density. $F_i$ is the fluid–solid interaction force. Firstly, virtual solid lattices, which are the row of lattice nodes nearest to fluid nodes, are assigned a specific chemical potential which indicates the surface wettability. The density of virtual solid lattice is the average density of fluid nodes adjacent to virtual solid lattice. Using the specified chemical potential and the density of virtual solid lattice finally can evaluate the interaction force $F_i$ by using Eq. (6) again. $F_b$ is the body force,

$$F_b(x,t) = \rho(x,t)g,$$

where $g$ is the gravity acceleration. The force $F$ is introduced into the evolution equation of the lattice Boltzmann model by using a widely used interparticle interaction proposed by Shan-Chen [8]. Thus, the equilibrium velocity $u^{eq}$ and the macroscopic fluid velocity $v$ are revised as

$$u^{eq} = u + \tau \delta \frac{F}{\rho}, \quad v = u + 0.5\delta \frac{F}{\rho}.$$

Therefore, the corresponding evolution equation of the lattice Boltzmann model is redefined as

$$f_i(x + e_i \delta t + \delta t) - f_i(x,t) = -\frac{1}{\tau} \left[ f_i(x,t) - f_i^{(eq)}(\rho, u^{eq}) \right],$$

where the equilibrium density distribution function still takes Eq. (2).

In these simulations, the Peng–Robinson (PR) EOS is chosen to describe the fluid, which shows superior in predicting liquid densities. The PR EOS is given by [9]

$$p_0 = \frac{\rho RT}{1 - b \rho} - \frac{a \alpha(T) \rho^2}{1 + 2b \rho - b^2 \rho^2},$$

where the temperature function is:

$$\alpha(T) = [1 + (0.37464 + 1.54226 \omega - 0.26992 \omega^2) \times (1 - \sqrt{T/T_c})^2]$$

and $\omega$ is the acentric factor, which is equal to 0.344 (the acentric factor of water), the critical temperature is $T_c = 0.072919$, and the critical density is $\rho_c = 2.657304$, the attraction parameter takes $a = 9/49$, and the volume correction takes $b = 2/21$, the universal gas constant is $R = 1$ [10].

3. Model validation

3.1. Coexistence density curves

As the most important thermodynamic consistent test, the coexistence density curve of the fluid system with PR EOS is calculated and compared with those predicted by the Maxwell equal-area construction [11]. The parameters used in our simulations are chosen as follows: the computational domain is $N_x \times N_y \times N_z = 160^3$ lu (lu represents lattice unit, the same unit for the following), and a spherical droplet with a radius of $r_0 = 30$ is initially placed at the center of the domain. Periodic boundary conditions are applied on the solid surfaces. The density field is initialized as

$$\rho(x,y,z) = 0.5(\rho_l + \rho_s) - 0.5(\rho_l - \rho_s) \times \tanh \left[ \frac{2 \sqrt{(x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2} - r_0}{W} \right],$$

where the thickness of the interface is $W = 5$. In order to relate the numerical results to the real physical properties, we define the reduced temperature $T_T = T/T_c$ and reduced density $\rho_r = \rho/\rho_c$. The
present numerical simulations are consistent with the analytical solutions in both gas branch \((\rho_r < 1)\) and liquid branch \((\rho_r > 1)\), as shown in Fig. 1(a). It indicates that the model used in this work is capable of achieving thermodynamic consistency.

Figure 1. (a) Two-phase coexistence curve of PR EOS, (b) pressure difference vs. \(1/R\).

3.2. Laplace’s law

Laplace’s law is usually used to verify the accuracy of a multiphase flow model [12]. From the Laplace’s law, the relationship between the pressure difference \(\Delta P\) and the final radius of droplet \(R\) yields the expression as [13]

\[
\Delta P = 2\sigma / R, \tag{12}
\]

where \(\sigma\) is the surface tension, \(\Delta P = P_{\text{in}} - P_{\text{out}}\) is the pressure difference between the inside and outside of droplet. Fig. 1(b) shows the relationship between \(\Delta P\) and \(1/R\) at different temperatures. As the temperatures are \(Tr = 0.77, 0.80\) and \(0.84\), the radius of the droplets are \(R = 25, 30, 35, 40, 45\) and \(50\), respectively. It can be seen that Laplace’s law is well satisfied in the test, confirming the present model can capture the phase interface correctly.

4. Results and discussion

In this section, the present model described in Section 2 is implemented to simulate the process of coalescence-induced droplet jumping on pillared SHSs, which is structured with regularly spaced pillars. The pillars have height \(H = 6\), width and length \(L = 4\), and the distance between two consecutive pillars \(D = 8\). The contact angle between the droplet and the pillared surface is \(\theta = 153^\circ\), and different contact angles can be obtained through endowing the SHS with a specific chemical potential [7]. The computational domain is \(Nx \times Ny \times Nz = 192 \times 160 \times 160\) with halfway bounce-back boundary condition for all the solid surfaces. The parameters are fixed at density of gas \(\rho_g = 0.1970788\), density of liquid \(\rho_l = 7.2040512\), reduced temperature \(Tr = 0.80\), coefficient of surface tension \(\kappa = 0.02\), the acceleration of gravity \(g = 7 \times 10^6\). The radius of droplets is initially \(R = 20\), the interval between the droplets is \(6\), and the thickness of the interface layer is \(W = 5\). All corresponding parameters of the following simulations are the same as those above unless otherwise specified.

4.1. The coalescence-induced jumping of two droplets

4.1.1. Effect of pillar distance. Fig. 2 presents the coalescence-induced jumping process of two droplets on a SHS. At the beginning, two droplets are placed on the pillared SHS (\(t = 0\)). Owing to interfacial tension of droplets, droplets move slowly towards each other during the initial period. Then a tiny liquid bridge is formed between droplets and expands rapidly (\(t = 200\)). Thereafter the coalescing droplet forms a dumbbell shape followed by capsule shape (from \(t = 400\) to \(600\)), and further becomes approximate spherical shape (\(t = 800\)). The coalesced droplet jumps away from the pillared SHS due to the excess
surface energy released by the coalescence of two droplets. While moving in upward direction, the detached droplet, which could be affected by various potential energy, such as upward kinetic energy and gravitational potential energy, starts oscillation between the oblate and prolate shapes (from t=1000 to 1400). Finally, the coalesced droplet approaches to a spherical shape (t=4000), after several oscillations.

**Figure 2.** The simulated coalescence-induced jumping process of two droplets. The distance of the pillars is D = 3.

We set different distance of the pillars to investigate the pillared SHS which affects the jumping height of the coalesced droplet. The comparison of jumping height of the coalesced droplets on the different pillared SHSs, which is structured with different distance between the pillars (D=3, 11 and 19), is showed in Fig.3. As shown in Fig.3, for the same size of droplets, the jumping height of the coalesced droplet gradually decreases with the increase of the distance between pillars, in accordance with previous literature results[14]. The main reason for this phenomenon is that the larger the distance between pillars is, the more likely the coalesced droplets will be filled of the pillared gap, which could increase the surface wettability. As a result, the resistance of the movement of the three-phase contact line during the bottom radius contraction of the coalesced droplets increases, which will affect the jumping height of the coalesced droplets.

**Figure 3.** Comparison of jumping height of the droplets on pillared surfaces.

To enhance the persuasiveness of the conclusion, we further study the effect of the distance between pillars on the jumping height of the coalesced droplet at different droplet radii (from 12 to 36 at intervals of 2). Fig.4(a) shows the dependence of the droplet jumping height on the droplet radius for different distance between pillars (D=3, 11 and 19). We confirm again that, for the same radius of the droplets, the jumping height of the coalesced droplet becomes lower with increasing distance between pillars. Furthermore, the jumping height of the coalesced droplet gradually decreases with increasing radius of the droplets while keeping the other conditions fixed. The main reason for this phenomenon is that the released excess surface energy by the coalesced droplet needs to overcome more gravitational potential energy and more surface adhesion than the small coalesced droplet.

In order to fully reflect the effect of the distance between pillars on droplet jumping behavior, a series of simulations are carried out. As shown in Fig.4(b), there is the distribution of coalescence-induced jumping of two droplets with the radius of droplets changed from 12 to 38 at intervals of 2 and the distance of pillars changed from 3 to 39 at intervals of 3. From Fig.4(b), the coalesced droplets can jump on SHSs with a relatively small radius of the droplets less than 38 and distance of the pillars less than 40. In other words, the smaller the droplet radius and the distance of the pillars, the more likely the droplet would jump.
4.1.2. Effect of pillar height. Fig. 5(a) shows the dependence of droplet jumping height on droplet radius for different height of the pillars (H=5, 7 and 10). The result shows that, for the same radius of droplets, the larger the height of the pillars is, the higher the droplet jumping height is, which is in accordance with previous studies [14]. Moreover, for the same pillared height, the jumping height of the droplet decrease with the increase of droplet radius, the reasons of which is the same as in Fig. 4(a). As Fig. 5(b) shows, there is the distribution of coalescence-induced jumping of two droplets for different radii of droplet (from 12 to 40 at intervals of 2) and height of the pillars (from 1 to 10 at intervals of 1). The coalesced droplets can only jump on SHSs with a relatively small radius of droplets less than 36 and height of the pillars greater than 1. The results indicate that the smaller the droplet radius and the larger the height of the pillars are, the more likely the coalesced droplet jump. It is noted that the droplets cannot jump when the height of the pillars is equal to 0. The result for the coalesced droplet on flat surface is consistent with those obtained by Shi et al. [15].

4.1.3. Effect of surface contact angle. Under different contact angles, the jumping height of droplets with different radii taking the values of R=16, 18, 20 and 24, respectively, is shown in Fig. 6(a). Fig. 6(a) clearly shows that, for droplets with different radii, the jumping height of the coalesced droplet increases rapidly as the contact angle increases, but when the contact angle increases to a certain extent (θ = 140º), the growth rate of the jumping height of the coalesced droplet begins to slow down; and for the same contact angle, the smaller the droplet radius, the higher the jumping height of the coalesced droplet. Fig. 6(b) shows the distribution of coalescence-induced jumping of two droplets for different radii of droplets (from 12 to 36 at intervals of 2) and contact angles (from 126º to 165º at intervals of 3º). The coalesced droplet can only jump on pillared surfaces where the radius R is relatively small (less than 36) and the contact angle is relatively large (greater than 132º), as shown in Fig. 6(b). In a word, the droplet is more likely to jump with larger surface contact angle and smaller radius of droplets.
4.2. The coalescence-induced jumping of multidroplet

The above simulations is only for the coalescence-induced jumping of two droplets, however, in reality, more situations are the coalescence and jumping of multiple droplets [5]. Therefore, this section investigates the effect of the number of droplets on the droplet coalescence and jumping. The simulation domain is \( N_x \times N_y \times N_z = 224^3 \), multiple equally sized droplets are initially placed on the SHS. The droplet evolution during jumping induced by coalescence of two, three, four and five droplets is shown in Fig.7. The spontaneous jumping process about multidroplet is qualitatively similar with that of two droplets. However, there still exist some differences. As the number of droplets increases, the time of establishing the liquid bridge, forming the spherical shape and coalesced droplets jumping to the highest position is different, and the more coalescing droplets, the longer it takes.

As shown in Fig.8, we find that the droplet jumping height will increase and then decrease with the increasing of the droplet number. Moreover, we notice that, in our simulated results, the coalesced droplet always can jump to the highest position when the coalescing droplet number is 4. To understand the phenomena, some theoretical analyses below are given. In general, the more droplets merge, the greater the excess surface free energy released by droplet coalescence and the higher the jumping height of the coalesced droplet. Nevertheless, when the number of droplets is too large (such as \( N = 5 \)), the jumping height of the coalesced droplet begins to decline. The main reason for this phenomenon is that the more droplets merge, the more obvious the effect of gravity obstruction is, which affects the jumping height of the coalesced droplet.

Fig.8 shows the dependence of the droplet jumping height on the distance between two pillars, the height of the pillars and the contact angle for the number of droplets \( N = 2, 3, 4 \) and 5, respectively. From Fig.8 (a), we observe that, regardless of the number of droplets, the jumping height of the
coalesced droplet decreases as the distance of the pillars increases, for the same reason as described above in Fig.3. The jumping height of the coalesced droplet will increase as the pillar height increases, as presented in Fig.8 (b). Besides, the results also indicate that, regardless of the number of coalescing droplets, the droplet jumping height will increase as the contact angle increases. It is noted that, when the contact angle is larger than jumping critical contact angle, the droplet jumping height increases rapidly with the contact angle increase within a relatively small range of contact angles; when the contact angle continues to increase to a certain extent, the growth rate of the droplet jumping height tends to be flat.

Figure 8. Dependence of the droplet jumping height on (a) the distance of the pillars D, (b) the height of the pillars H and (c) the contact angle.

5. Conclusion
In this work, the coalescence-induced droplet jumping on SHSs is comprehensively and systematically studied in details by using a three-dimensional chemical-potential-based multiphase lattice Boltzmann model. In order to investigate the influence of pillared SHSs (height and distance of the pillars), the contact angle, the number and the size of droplets on droplet behaviors, the coalescence and jumping of two droplets and multidroplet are simulated and analyzed, respectively. The coalesced droplet can jump only under appropriate droplet size and characteristic parameters of SHSs. In addition, coalesced droplets are more likely to jump and jump higher on SHSs with larger contact angle and height of the pillars and smaller distance between two pillars. As the number of coalescing droplets increases, the droplet jumping height will increase and then decrease. The main reason for this phenomenon is that the more droplets merge, the more obvious the effect of gravity obstruction is, which affects the jumping height of the coalesced droplet. In our simulation, the coalesced droplet can jump to the highest position when the number of droplets is 4. The extension of this work considering effects of detailed microstructure with a more accurate three-dimensional multi-relaxation-time Chemical-Potential lattice Boltzmann simulation on coalescence-induced droplet jumping is in progress.

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