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# STUDY ON DROPLET NUCLEATION POSITION AND JUMPING ON STRUCTURED HYDROPHOBIC SURFACE USING THE LATTICE BOLTZMANN METHOD

by

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In this study, droplet nucleation and jumping on the conical micro-structure surface is simulated using the lattice Boltzmann method. The nucleation and jumping laws of the droplet on the surface are summarized. The numerical results suggest that the height and the gap of the conical micro-structure exhibit a significant influence on the nucleation position of the droplet. When the ratio of height to the gap of the micro-structure (H/D) is small, the droplet tends to nucleate at the bottom of the structure. Otherwise, the droplet tends to nucleate towards the side of the structure. The droplet grown in the side nucleation mode possesses better hydrophobicity than that of the droplet grown in the bottom nucleation mode and the droplet jumping becomes easier. Apart from the coalescence of the droplets jumping out of the surface, jumping of individual droplets may also occur under certain conditions. The ratio of the clearance to the width of the conical micro-structure (D/F) depends on the jumping mode of the droplet. The simulation results indicate that when the D/F ratio is greater than 1.2, the coalescence jump of droplets is likely to occur. On the contrary, the individual jump of droplets is easy to occur.

Key words: droplet, micro-structure, droplet nucleation position, droplet jumping, lattice Boltzmann method

## Introduction

According to the wettability of vapor condensation of droplets on the solid surface, it can be categorized as filmwise condensation and dropwise condensation. Dropwise condensation with a quite higher heat transfer coefficient compared with filmwise condensation [1-3], which had great potential in various fields of industrial production, such as steam power in industry, seawater desalination, thermal power plant, petrochemical industry and so on [4, 5]. Enhanced dropwise condensation heat transfer attracted more attention by researchers over recent years [6]. In dropwise condensation, rapid removal of droplets from the surface is a crucial way to improve the heat transfer performance [7]. Hydrophobic or super-hydrophobic surface modified with micron or nanometer structure was used as the base to study the condensation of droplets. The condensation heat transfer efficiency was found to be

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improved by adopting the methods like increasing the contact angle of a droplet [8-10]. Mishchenko *et al.* [11] studied the influence of dynamic droplets on supercooling behavior on the surface of micro-structure. Zhu *et al.* [12] prepared a super-hydrophobic surface using the nanoneedle cluster structure, which can generate the upward Laplace pressure to drive the droplet to move upward. By controlling the growth time, Wang *et al.* [13] prepared ZnO nanocecs of different height, diameter, and spacing. The influence of structure parameters on the heat transfer coefficient of surface condensation was obtained using theoretical analysis and experimental verification. The influence of the basic shape of the wettability of the solid surface is studied by Checco *et al.* [14]. It was observed that the conical structure has better hydrophobicity than the columnar structure and is more easily obtained in the experimental preparation. Hence, it is of practical value to study the influence of conical micro-structure on droplet condensation.

Boreyko *et al.* [15] was the first one to report a new phenomenon of condensation droplets jumping on the super-hydrophobic surface. Since then, this condensation had received a lot of attention [16-18]. Although a variety of experiments have been conducted in this field [19, 20], it is difficult to accurately achieve the expected surface structure through experiments. Also, the relationship between surface droplet behavior and surface micromorphology cannot be established precisely. The simulation study is not limited to the conditions of preparation and condensation in the laboratory, which is conducive to the mechanism analysis and prediction of condensation. Therefore, researchers preferred to use numerical simulation to estimate the condensation and jump of droplets [21].

The lattice Boltzmann method (LBM) was a CFD method with significant superiority developed in the past couple of decades. Mesoscopic LBM breaks through the limitations of traditional macro CFD method, it considers the interaction between particles in the process of phase separation and interfacial evolution, and can deal with complex boundary conditions. The LBM has exhibited significant potential in the study of multiphase flows and is suitable for simulating the complex processes of droplet nucleation, growth, coalescence, and jumping. Hence, it was widely used in the study of multiphase flow and wettability [22, 23]. Eventually, LBM was adopted to study the droplet migration and nucleation on the surface of the structure [24-26]. Shi *et al.* [27] used a 3-D lattice Boltzmann model to examine the vertical coalescence jumping and horizontal movement of the droplets on the surface with different micro-structure arrays.

In the previous researches, the simulation was primarily based on the surface model of the cylindrical structure. The simulation of the surface of the conical micro-structure was indeed rare. Nevertheless, the specific structural characteristics of the conical surface may have different effects on the condensation process of the droplet. In this study, a multiphase, multicomponent LBM model on account of the Shan-Chen scheme was used to study the nucleation, growth and jumping of droplets on conical micro-structure surface. The effects of geometric parameters such as the gap, height and width of the surface micro-structure on the preferential nucleation position and jumping phenomenon of condensed droplets were studied, and the relationship between the geometry of the conical surface and the droplet growth and movement was revealed.

#### Numerical method

In LBM simulation, the motion of the fluid can be represented by the density distribution function. Using BGK collision operator, the standard lattice Boltzmann equation with force terms can be expressed:

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

where k = 1, 2 and i = 1, 2, ..., 8.  $f_i^k(x, t)$  is the component density distribution function, including water vapor and other non-condensable gases [21]. The  $\tau^k$  is the relaxation time of the  $k^{\text{th}}$  component. The  $\delta_t$  is the time step. The  $e_i$  is discrete velocities in the D2Q9 model are given by:

$$e_i = \begin{cases} (0,0), & i = 0\\ (\pm 1,0), & (0,\pm 1), & i = 1 \sim 4\\ (\pm 1,\pm 1), & i = 5 \sim 8 \end{cases}$$
(2)

The  $f_i^{k(eq)}(x, t)$  is the equilibrium distribution function expressed by:

$$f_i^{k(\text{eq})}(x) = \omega_i \rho^k(x,t) \left\{ 1 + \frac{3[e_i u^k(x,t)]}{c_s^2} + \frac{4.5[e_i u^k(x,t)]^2}{c_s^4} - \frac{1.5[u^k(x,t)]^2}{2c_s^2} \right\}$$
(3)

The weight coefficients  $\omega_i$  are given as:

$$\omega_{i} = \begin{cases} \frac{4}{9}, & e_{i}^{2} = 0\\ \frac{1}{9}, & e_{i}^{2} = c^{2}\\ \frac{1}{36}, & e_{i}^{2} = 2c^{2} \end{cases}$$
(4)

where  $\rho^k$  is the macroscopic density of the  $k^{\text{th}}$  component, which can be obtained by:

$$\rho^{k}(x,t) = \sum_{i=0}^{8} f_{i}^{k}(x,t)$$
(5)

The macroscopic velocity  $u^{k(eq)}(x, t)$  is given by:

$$u^{k(eq)}(x,t) = u'(x,t) + \frac{\tau^{k} \delta t F^{k}(x,t)}{\rho^{k}}$$
(6)

where  $F^{k}(x, t)$  is the force acting on the  $k^{\text{th}}$  component, which includes the fluid-fluid cohesion force  $F^{k}_{n}(x, t)$  and the fluid-solid adhesion force  $F^{k}_{ads}(x, t)$ :

$$F^{k}(x,t) = F^{k}_{n}(x,t) + F^{k}_{ads}(x,t)$$
(7)

The fluid-fluid cohesive force acting on the  $k^{\text{th}}$  component is defined:

$$F_{n}^{k}(x,t) = -\psi^{k}(x,t) \sum G(x,x') \sum_{i} \psi^{\bar{k}}(x',t) e_{i}$$
(8)

where *k* and  $\overline{k}$  represent two different fluid components,  $\psi^k(x, t)$  and  $\psi'(x', t)$  are the pseudo potentials that are commonly taken as fluid densities:  $\psi^k(x, t) = \rho^k(x,t)$ , and  $\psi^{\overline{k}}(x,t) = \rho^{\overline{k}}(x,t)$ . The G(x, x') is a parameter that controls the strength of the cohesion force is given by:

$$G(x, x') = \begin{cases} G, & |x - x'| = c \\ \frac{G}{4}, & |x - x'| = \sqrt{2}c \\ 0, & \text{otherwise} \end{cases}$$
(9)

The values of pressure at different positions can be expressed:

$$P(x,t) = \frac{\sum_{k} \rho^{k}(x,t)}{3} + \frac{G}{3} \psi^{k}(x,t) \psi^{\bar{k}}(x,t)$$
(10)

The fluid-solid adhesion force acting on the  $k^{\text{th}}$  component is:

$$F_{\text{ads}}^{k}(x,t) = -\rho^{k}(x,t) \sum \omega_{i} G_{\text{ads}}^{k} s(x+e_{i}\delta t,t)e_{i}$$
(11)

where s is the wall index, which is 1 when the lattice property is solid, and 0 when the lattice property is fluid. The interaction strength between the fluid and solid phases can be adjusted by  $G_{ads}^k$ .

#### **Results and discussions**

#### Model validation

#### Laplace validation

To validate the previously mentioned model, its Laplace law is tested first. According to Laplace's law, the pressure change inside and outside the droplet is linearly related to the inverse of the droplet radius, and the slope is the surface tension. For a liquid drop at rest, Laplace's law can be expressed:

$$p_{\rm in} - p_{\rm out} = \Delta p = \frac{\sigma}{r} \tag{12}$$

where  $p_{in}$  and  $p_{out}$  represent the average pressure inside and outside the droplet, respectively,  $\Delta p$  – the difference between the internal and external average pressure of the droplet,  $\sigma$  – the surface tension coefficient, and r – the radius of the droplet. First, the calculation domain is set to 101×101 lu (lattice unit), in its central (50, 50) set static droplets. The boundaries around the calculation domain are set as the periodic boundary conditions, ignoring the influence of gravity, and the radius of the droplets, 5.0, 10.0, 15.0, 20.0, and 25.0 grid length, respectively. Simulated by altering the droplet radius and record of the different radius of droplet Laplace pressure, then compute the droplet pressure difference inside and outside  $\Delta p$ . The  $\Delta p$  possesses a linear relationship with 1/r, which expected from the Laplace's law. The slope is the surface tension that can be calculated using the formula. Figure 1(a) demonstrated the  $\Delta p - 1/r$  fitting curve when G = 0.4, and it can be concluded that the fluid surface tension is about 0.2112 at this time.

#### Verification of contact angle

In the Shan-Chen model, given the interaction intensity, G, between the fluid particles, different contact angles can be calculated by adjusting  $G_{ads}^k$ . The fluid-solid interaction strength,  $G_{ads}^1$  (H<sub>2</sub>O/solid) and  $G_{ads}^2$  (non-H<sub>2</sub>O gases/solid), are set to  $G_{ads}^1 = -G_{ads}^2$ . The calculation domain is set as 101×101 lu during the simulation. The bounce-back condition is ap-

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plied at the bottom and top boundaries, and the left and right boundaries are observed to be periodic. Initially, the droplet with a radius of 15 lu is placed at the bottom, and the code is run to equilibrium. Figure 1(b) indicates the relationship between the contact angle and the strength of fluid-solid interaction  $G_{ads}^1$ , the contact angle increases linearly with  $G_{ads}^1$ , which consistents with the previous report [28]. It proves that the model can be employed to simulate the dynamic process of droplet condensation and surface wetting.



Figure 1. Model validation; (a) relationship between capillary pressure and droplet radius and (b) dependence of contact angle on strength coefficient  $G_{ads}^1$  value

## Setting of simulation parameters and initial conditions

The geometry size of the conical micro-structure on the rough surface incorporates four parameters: The W indicates the bottom width of the single conical micro-structure, F – the top width, D – the conical pitch of the micro-structure, and H – the height of the conical micro-structure, as represented in fig. 2(a). The H/D represents the ratio of height to clearance of the micro-structure, and D/F represents the ratio of the clearance to the width of the conical micro-structure. In the presented work, the influence rule of the conical microstructure geometry size on the condensation droplet nucleation position and jumping is simulated to examine the setting of regional boundary conditions by modifying the aforementioned parameters, as represented in fig. 2(b). The bounce-back condition is used for the bottom boundary, a periodic boundary is applied at the left and right boundaries, and the Zou-He [29] pressure condition is applied at the top boundary to furnish steam to the system.



Figure 2. Simulated variables and conditionals; (a) conical micro-structure and (b) boundary conditions

In this paper, the simulation system is filled with water vapor (H<sub>2</sub>O) and other noncondensable gases (non-H<sub>2</sub>O). The initial gas component density parameters are set as follows:  $\rho_{\rm H_2O} = 0.01 \text{ mu/lu}^2$  (mass units per square lattice unit) and  $\rho_{\rm non-H_2O} = 0.99 \text{ mu/lu}^2$ . The parameters of gas components continuously injected into the system from the top boundary stay in  $\rho_{\rm H_2O} = 0.04 \text{ mu/lu}^2$  and  $\rho_{\rm non-H_2O} = 0.99 \text{ mu/lu}^2$ . The interaction intensity between fluid particles is set as G = 0.4 and the fluid-solid interaction strength,  $G_{\rm ads}^1$  (H<sub>2</sub>O/solid) and  $G_{\rm ads}^2$ (non-H<sub>2</sub>O gases/solid), are set as  $G_{\rm ads}^1 = -G_{\rm ads}^2 = 0.03$ . Convergence accuracy of pressure set to  $1.0 \cdot 10^{-6}$ .

## Simulation of droplet nucleation position

Figure 3(a) demonstrates the simulation results of the droplet nucleation process on the bottom surface of the conical micro-structure. The calculation domain is set to  $180 \times 101$  lu, and the remaining boundary conditions are mentioned in section *Setting of simulation parameters and initial conditions*. The geometric dimensions of the conical micro-structure were set as: W = 22 lu, F = 10 lu, D = 8 lu, and H = 12 lu. In fig. 3, the color indicates the density of water vapor. The density of water vapor gradually increases from blue to red and eventually condenses into droplets. It can be noticed from fig. 3(a) that the density of the water component in the gas phase increases gradually as the LBM simulation begins. During the initial stages of condensation, the water molecules in convex cone structure gaps gathered themselves at t = 3000, and the enrichment of water vapor in the bottom formed a thin layer of the liquid membrane at t = 4400. Droplet nucleation in gap base conical micro-structure is raised after t = 5200, followed by the absorption of water molecules in the surrounding gas phase. Nevertheless, the droplets grow beyond the height of the conical micro-structure at t = 10000. Comparing the three typical nucleation modes of columnar surface proposed by Zhang *et al.* [26], the droplet nucleation mode is identified as the bottom nucleation mode of conical micro-structure.



**Figure 3.** Nucleation modes of droplet on structural surface; (a) the bottom nucleation model of condensate droplet and (b) the side nucleation model of condensate droplet (for color image see journal web site)

Figure 3(b) represents the simulation results of the droplet nucleation process on the sides of the conical micro-structure surface. The calculation domain is consistent with figure 3(a). The geometric dimensions of the conical micro-structure were set as: W = 22 lu, F = 10 lu, D = 8 lu, and H = 18 lu. It can be observed from fig. 3(b) that the density increases gradually at the beginning of the simulation. In the water component in the gas phase at t = 3000, the water molecule is gathered by the clearance between the convex cone micro-

structure. At t = 5200, the droplet core begins in the sides of the conical micro-structure and droplets start to appear in the clearance side of the conical micro-structure. The water molecules in the surrounding gas phase growth get absorbed after t = 6200. The droplet nucleation model is known as the side nucleation model of conical micro-structure, according to the research by Zhang *et al.* [26]. Tiny droplets on the side of adjacent structures are combined to form larger droplets at t = 10000, and the droplets tend to move up along the gaps.

There are two droplet nucleation modes of bottom nucleation and side nucleation will appear while changing the height of the conical structure as demonstrated in figs. 3(a) and 3(b). The H/D are related to the nucleation position of the droplet after more groups of similar simulations. The bottom nucleation is more likely to occur on the surface of the structure with a larger ratio, whereas the side nucleation occurs easily with a smaller ratio. With the growth of the droplets, the droplets generated in the bottom nucleation mode fill the bottom gap and eventually spill over the surface. Evidently, this structure can weaken the hydrophobicity of the surface of the micro-structure. In the side nucleation mode, the droplet will move upward along the gap to form a stable Cassie state. At this point the surface seems more hydrophobic and is conducive to enhancing the condensation heat transfer efficiency of the droplet.

## Simulation of droplets jump modes

Figure 4(a) indicates the simulation results of individual droplets jumping process on the surface of the conical micro-structure. The dimension of the simulated area is  $168 \times 101$  lu, and the geometric size of the conical micro-structure was set as: W = 22 lu, F = 5 lu, D = 6 lu, and H = 18 lu. The boundary conditions of the model are highlighted in section Setting of simulation parameters and initial conditions. The color in fig. 4 represents the same meaning as that in fig. 3, representing the density of water molecules. As illustrated in fig. 3, the colors in fig. 4 also represent the density of water vapor. The droplet nucleation model is side nucleation and the simulation results before t = 5000 are nearly consistent with the side nucleation process above. In the following calculation, individual droplets in adjacent clearance constantly propagate upward along with the structural clearance under the action of the upper and lower pressure difference. At t = 7000, individual droplets in principal from the side of the structure rise up to the top. Moreover, with the growth of a droplet in this process, the droplet radius reaching the top can be recorded to increase significantly. Later, as the droplets continue to grow and move, the droplets in the gaps between the adjacent conical micro-structures ultimately separate from the bottom structure at t = 7600, the individual droplets in the gaps can jump at this point. While the bottom surface is far away from the liquid phase, it is difficult to absorb the water molecules in the gas phase by the liquid phase and the droplet starts to nucleate at the bottom gap. Studies on individual droplet jump can be verified through the previous research [30]. The droplet moves above the gap due to the difference in capillary pressure between the bottom and top of the droplet. In fact, in this case, the coalescence is not necessary for the droplet jumping. The energy released when an individual droplet deforms because of departure from the structure is enough to cause the droplet to jump.

Figure 4(b) indicates the simulation results of droplets by coalescence jumping out from the surface. The size of the simulated area is  $175 \times 101$  lu, and the geometric dimension of the conical micro-structure was set as: W = 22 lu, F = 5 lu, D = 7 lu, and H = 18 lu. Specific simulation conditions are consistent with the previous conditions. This result of the simulation is similar to that in fig. 4(a). The water vapor nucleates on the sides of the structure and coalesces to form a larger droplet. In the following simulation, the droplet in the adjacent clearance moves upwards along the structural clearance under the action of the pressure dif-



**Figure 4.** The jump modes of the droplet; (a) individually jump of droplet and (b) coalescence jump of droplet (for color image see journal web site)

ference between the bottom and top of the droplet. At t = 8600, the droplets propagate up from the micro-structure gaps to the top, which is different from the individual droplet jumping off the surface in fig. 4(a). Since the gap of the adjacent conical structure in fig. 4(b) is larger than that in fig. 4(a), the droplet radius generated after reaching the top of the gap is also larger. After individual droplets move up to top breakthrough the limitation of conical micro-structure top width, the droplets coalescence occur at t = 9400. The contact area between the droplets and the surface becomes smaller during the process of the droplet by coalescence. With the release of surface free energy, droplets jump off the surface due to excess kinetic energy. As illustrated at t = 10200, the coalescence jump of the droplet is realized. After that, the results were similar to fig. 4(a). Since the bottom surface is far away from the liquid phase and there are more water molecules in the gas phase, the droplet begins to nucleate at the bottom gaps.

As shown in figs. 4(a) and 4(b), there are two droplet jump modes of individually jump and coalescence jump appear when the gap between adjacent conical micro-structures on the bottom surface change. The D/F is related to the droplet jumping mode. In general, the smaller the ratio of clearance to top surface width is, the more likely it is to jump an individual droplet. Whereas for larger ratios, droplet coalescence jump is easy. The simulation results prove that when D/F > 1.2, the coalescence jump of droplets is likely to occur, an individual jump of the droplet is easy to occur.

## Conclusions

In this paper, the condensation of droplets on the hydrophobic surface of the conical micro-structure was studied using a 2-D multicomponent multiphase flow LBM model. The influence rule of the conical micro-structure geometry size on the nucleation position and jumping of the condensing droplets was explored. The conclusions are as follows.

- The *H/D* depends on the nucleation position of the droplet. A small ratio is favorable for nucleation at the bottom of the structure and a large ratio is favorable for nucleation at the side of a conical micro-structure. The droplet grown in the side nucleation mode exhibits better hydrophobicity than the droplets grown in the bottom nucleation mode and is more conducive to condensation heat transfer of droplet.
- The larger the gap of the conical micro-structure, the larger the droplets formed in the gaps, and conversely, the smaller the gaps, the smaller the droplets formed. The D/F is related to the jumping mode of the droplet. The smaller the ratio is, the more likely it is to jump an individual droplet. When the ratio is larger, it is easy for the droplets to coalesce and jump. Simulation results indicate that when D/F is greater than 1.2, the coalescence jump of the droplet is likely to occur. Otherwise, the individual jump of the droplet is easy to occur.

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#### Nomenclature

c – sound velocity [ms <sup>-1</sup> ]	$\rho$ – density [kgm <sup>-3</sup> ]
e – discrete velocities [ms <sup>-1</sup> ]	$\tau$ – relaxation time [s]
F – force [N] G – force coefficient	Subscripts
P – pressure [Pa]	i – discrete direction
s – wall index u – macroscopic velocity [ms <sup>-1</sup> ]	Superscripts
Greek symbols	$k - k^{\text{th}}$ component

 $\delta$  – the time step

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