



Technical Note

Lattice Boltzmann simulations for self-propelled jumping of droplets after coalescence on a superhydrophobic surface



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ABSTRACT

The phenomenon of coalescence induced droplets self-propelled jumping on superhydrophobic surfaces (SHS) is numerically simulated in this paper using 2D lattice Boltzmann method (LBM). To overcome numerical instability problems of a two-phase flows with a high liquid/vapor density ratio and a high liquid/vapor viscosity ratio, the equation of state is modified according to an existing method and the multiphase relaxation time (MRT) method is adopted. The simulated jumping velocity and jumping height of droplets with different radii are found in good agreement with experimental observations. In addition, the reason why coalescence droplets will jump on superhydrophobic surface with a sufficiently high contact angle is explained based on a qualitative analysis.

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1. Introduction

Droplets dynamic behaviors, such as coalescence and movement, play important roles in dropwise condensation process. Recently, a series of experimental studies [1–3] have been carried out on dropwise condensation on a superhydrophobic surface (SHS), which is associated with large contact angle ($>150^\circ$) and small hysteresis. In particular, Boreyko and Chen [1] performed the first droplet coalescence induced self-propelled jumping experiment on SHS, and measured jumping velocities for droplets with radius ranging from 10 μm to 150 μm . They assumed that all of released surface energy after droplet coalescence is converted to kinetic energy of the merged droplet and computed the jumping velocity of the droplet, which was compared with their measurements. Most recently, some analyses [4–6] have been carried out to study the mechanism of droplet jumping from a SHS. For example, Wang et al. [4] as well as Liu et al. [5] have improved the analysis by taking into consideration energy dissipation. Peng et al. [6] carried out an LB simulation on coalescence of two droplets based on the free-energy model [7] to determine the effective kinetic energy with the jumping height estimated based on this kinetic energy. However, the two droplets in their LB simulation were not in contact with the surface and no jumping motion was actually simulated.

In this Short Communication, we have carried out a lattice Boltzmann simulation based on the pseudo-potential LB model proposed by Shan and Chen [8] with real gas equation of state (EOS) taken into consideration. In order to obtain simulations applicable to high density ratios, we adopt the method proposed by Hu *et al.* [9], who modified the equation of state (EOS) $p = f(\rho, T)$ by multiplying a coefficient k ($k < 1$) such that $p' = kp = kf(\rho, T)$. It will be shown that this modification actually changes one parameter in the EOS. Furthermore, the MRT model [10] is adopted to improve the numerical instability associated with high liquid/vapor viscosity ratios in the physical problem. The simulated results for jumping velocity and jumping height of droplets with different radii are compared with experimental results of Boreyko and Chen [1].

2. Description of the simulation model

In this section, we will firstly introduce the pseudopotential multiphase LBM with MRT collision matrix. Then, we will show how physical parameters in an EOS are changed by the modification of Hu *et al.* [9].

2.1. MRT pseudopotential multiphase LBM

The density distribution evolution equation of LBM with the MRT collision operator is written as [10]

$$f_i(\mathbf{x} + \mathbf{e}_i \delta_t, t + \delta_t) - f_i(\mathbf{x}, t) = -\Lambda_{ij}(f_j(\mathbf{x}, t) - f_j^{\text{eq}}(\mathbf{x}, t)) + \Delta f_i(\mathbf{x}, t), \quad (1)$$

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where $f_i(\mathbf{x}, t)$ is the discrete distribution function for pseudoparticles moving with the discrete velocities \mathbf{e}_i at position \mathbf{x} and time t , $f_i^{eq}(\mathbf{x}, t)$ is its equilibrium distribution. And $\mathbf{A} = \mathbf{M}^{-1}\mathbf{S}\mathbf{M}$ is the collision matrix, in which \mathbf{S} is a non-negative diagonal matrix given by (for the D2Q9 lattice)

$$\mathbf{S} = \text{diag}(\tau_\rho^{-1}, \tau_e^{-1}, \tau_e^{-1}, \tau_j^{-1}, \tau_q^{-1}, \tau_j^{-1}, \tau_q^{-1}, \tau_v^{-1}, \tau_v^{-1}), \quad (2)$$

where τ is relaxation time. The kinematic viscosity of the fluid is $\nu = c_s^2(\tau_v - 0.5)\delta_t$.

And \mathbf{M} is an orthogonal transformation matrix [10]. Eq. (1) can be implemented between the projection of velocity space and moment space. Through the transformation matrix \mathbf{M} , the density distribution function f_i and its equilibrium distribution f_i^{eq} can be projected into the moment space as $\mathbf{m} = \mathbf{M}\mathbf{f}$, $\mathbf{m}^{eq} = \mathbf{M}\mathbf{f}^{eq}$, where the equilibria \mathbf{m}^{eq} is defined as

$$\mathbf{m}^{eq} = \rho \left(1, -2 + 3|\mathbf{u}|^2, 1 - 3|\mathbf{u}|^2, u_x, -u_x, u_y, -u_y, u_x^2 - u_y^2, u_x u_x \right)^T. \quad (3)$$

The collision step is implemented in the moment space as follows

$$\mathbf{m}' = \mathbf{m} - \mathbf{S}(\mathbf{m} - \mathbf{m}^{eq}), \quad (4)$$

where $\mathbf{f}' = \mathbf{M}^{-1}\mathbf{m}'$ is the distribution functions after collision.

The streaming process is

$$f_i(\mathbf{x} + \mathbf{e}_i\delta_t, t + \delta_t) = f_i'(\mathbf{x}, t) + \Delta f_i(\mathbf{x}, t). \quad (5)$$

where the force term $\Delta f_i(\mathbf{x}, t)$ is incorporated through the exact difference method (EDM) [11]

$$\Delta f_i(\mathbf{x}, t) = f_i^{eq}(\rho(\mathbf{x}, t), \mathbf{u} + \Delta\mathbf{u}) - f_i^{eq}(\rho(\mathbf{x}, t), \mathbf{u}), \quad (6)$$

with $\Delta\mathbf{u} = \mathbf{F} \cdot \delta_t / \rho$ being the velocity change due to the force term \mathbf{F} during time step δ_t . The density and velocity of the fluid are defined by

$$\rho = \sum_i f_i, \quad \rho\mathbf{u} = \sum_i \mathbf{e}_i f_i, \quad (7)$$

and the real fluid velocity is calculated as $\mathbf{U} = \mathbf{u} + 0.5\delta_t \cdot \mathbf{F} / \rho$.

The force term $\mathbf{F} = \mathbf{F}_{\text{int}} + \mathbf{F}_g + \mathbf{F}_s$, includes the interparticle interaction force \mathbf{F}_{int} , the gravitational force \mathbf{F}_g , and the interaction force between solid surface and fluid \mathbf{F}_s . The interparticle interaction force \mathbf{F}_{int} is given by Gong and Cheng [12] as

$$\mathbf{F}_{\text{int}} = -\beta\psi(\mathbf{x}) \sum_i G(\mathbf{x} + \mathbf{e}_i)\psi(\mathbf{x} + \mathbf{e}_i)\mathbf{e}_i - \frac{1-\beta}{2} \sum_i G(\mathbf{x} + \mathbf{e}_i)\psi^2(\mathbf{x} + \mathbf{e}_i)\mathbf{e}_i, \quad (8)$$

where β is the weight coefficient, $G(\mathbf{x} + \mathbf{e}_i)$ denotes the interaction strength, and $\psi(\mathbf{x})$ is the interaction potential given as

$$\psi(\mathbf{x}) = \sqrt{\rho c_s^2 - p}. \quad (9)$$

It is relevant to pointed out that Kupershtokh et al. [11] had also proposed an equation similar to Eq. (8) independently using a different approach. The gravitational force \mathbf{F}_g is calculated by

$$\mathbf{F}_g(\mathbf{x}) = (\rho(\mathbf{x}) - \rho_v)\mathbf{g}, \quad (10)$$

where \mathbf{g} is the acceleration of gravity and ρ_v is the density of the vapor phase.

The interaction force \mathbf{F}_s between solid surface and fluid is given by

$$\mathbf{F}_s = -G_s\rho(\mathbf{x}) \sum_i \omega_i s(\mathbf{x} + \mathbf{e}_i\delta_t)\mathbf{e}_i, \quad (11)$$

where G_s is the parameter denoting the fluid–solid interaction strength, and $s(\mathbf{x})$ is a binary function (with $s(\mathbf{x}) = 1$ for solid and $s(\mathbf{x}) = 0$ for fluid).

2.2. Parameters of EOS

The EOS can be incorporated into pseudopotential LBM models through Eq. (9), and the parameters in the EOS affect the numerical stability greatly. Hu et al. [9] modified the equation of state (EOS) $p = f(\rho, T)$ by multiplying a coefficient k ($k < 1$) such that $p' = kp = kf(\rho, T)$, and the modified model was shown to be able to simulate multiphase flow with higher value of liquid/vapor density ratio. This can be explained as follows.

The Peng–Robinson (P–R) equation of state is chosen to describe the fluid in this paper as

$$p = \frac{\rho R_g T}{1 - b\rho} - \frac{a\rho^2\alpha(T)}{1 + 2b\rho - b^2\rho^2}, \quad (12)$$

where R_g is gas constant, $\alpha(T) = [1 + (0.37464 + 1.54226\omega - 0.26992\omega^2)(1 - \sqrt{T/T_{cr}})]^2$, ω is the acentric factor and is equal to 0.344 in this work. The critical properties ρ_{cr} and T_{cr} depend on parameters R_g , a and b , which are given as,

$$\rho_{cr} = \frac{0.25342}{b}, \quad T_{cr} = \frac{0.170151a}{R_g b}. \quad (13a, b)$$

Substitute Eq. (13) into Eq. (12), and transform P–R EOS in terms of T_r (where $T_r = T/T_{cr}$ is the reduced temperature) as

$$p = a \left[\frac{0.170151\rho T_r}{b(1 - b\rho)} - \frac{\rho^2\alpha(T_r)}{1 + 2b\rho - b^2\rho^2} \right], \quad (14a)$$

and the modification proposed by Hu et al. [9] can be obtained as

$$p = k \left[\frac{\rho R_g T}{1 - b\rho} - \frac{a\rho^2\alpha(T)}{1 + 2b\rho - b^2\rho^2} \right] \\ = ka \left[\frac{0.170151\rho T_r}{b(1 - b\rho)} - \frac{\rho^2\alpha(T_r)}{1 + 2b\rho - b^2\rho^2} \right], \quad k < 1. \quad (14b)$$

Comparing Eqs. (14) and (15), the modification of Hu et al. [9] actually changes only the value of a , i.e., a smaller value of a is used. And since $\rho_{cr} = 0.25342/b$, it is clear that the Maxwell construction of density values (ρ_l and ρ_v) at the same T_r are not altered because the value of parameter b is unchanged. Using Hu's modification, it is possible to simulate problems with smaller values of T_r without encountering numerical instability.

Li et al. [13] also found a similar behavior using the Carnahan–Starling (CS) EOS. Similarly, we can obtain CS EOS, van der Waals (vdW) EOS and Redlich–Kwong (RK) EOS in the following forms

$$p = a \left[0.3773\rho T_r \frac{1 + b\rho/4 + (b\rho/4)^2 - (b\rho/4)^3}{(1 - b\rho/4)^3} - \rho^2 \right], \\ \rho_{cr} = \frac{0.5218}{b} \quad (\text{CS}) \quad (15a)$$

$$p = a \left[\frac{8\rho T_r}{27b(1 - b\rho)} - \rho^2 \right], \quad \rho_{cr} = \frac{1}{3b} \quad (\text{vdW}) \quad (15b)$$

$$p = a^{2/3} \left[\frac{0.34504\rho T_r R_g^{1/3}}{b^{2/3}(1 - b\rho)} - \frac{1.70242\rho^2 b^{1/3} R_g^{1/3}}{T_r^{0.5}(1 + b\rho)} \right], \\ \rho_{cr} = \frac{0.25992}{b} \quad (\text{RK}), \quad (15c)$$

Eqs. (14) and (15) show that Hu et al. proposed modification [9] change only the value of parameter a in these two constant EOS.

3. Results and discussion

In this section, we will firstly discuss the effect of contact angle on the kinetic energy of the coalescence droplet based on the

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