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Citation: [Physics of Fluids](#) **27**, 102102 (2015); doi: 10.1063/1.4932085

View online: <http://dx.doi.org/10.1063/1.4932085>

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Coalescence-induced jumping of droplet: Inertia and viscosity effects

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(Received 25 January 2015; accepted 12 August 2015; published online 6 October 2015)

The problem of coalescence-induced self-propelled jumping of droplet is studied using three-dimensional numerical simulation. The focus is on the effect of inertia and in particular the effect of air density on the behavior of the merged droplet during jumping. A lattice Boltzmann method is used for two identical, static micro-droplets coalescing on a homogeneous substrate with contact angle ranging from 0° to 180° . The results reveal that the effect of air density is significant on detachment of the merged droplet from the substrate at the later stage of the jumping process; the larger the air density, the larger the jumping height of the droplet. Analysis of streamlines and vorticity contours is performed for density ratios ranging from 60 to 800. These show a generation of vortical structures inside and around the droplet. The intensity of these structures gets weaker after droplet departure as the air inertia is decreased. The results are also presented in terms of phase diagrams of the merged droplet jumping for different Ohnesorge numbers (Oh) and surface wettabilities for both small and large density ratios. The critical value of contact angle where the merged droplet jumps away from the substrate is independent of density ratio and has a value around 150° . However, the critical value of Oh depends on both density ratio and wettability of the surface for contact angles greater than 150° . In this range of contact angle, the diagrams show two distinct dynamical regimes for different density ratios, namely, inertial and viscous regimes. © 2015 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4932085>]

I. INTRODUCTION

Coalescence-induced micro-droplet jumping has been demonstrated for various biological and industrial applications, including self-cleaning,¹ condensation heat transfer enhancement,^{2–5} anti-icing,^{6–8} anti-dew,^{9–11} and anti-corrosion.¹² This spontaneous removal from structured super-hydrophobic surfaces is achieved by converting surface energy to kinetic energy, independent of gravity.⁹ For droplet sizes comparable to or larger than the capillary length,^{13–15} self-propelled jumping has not been observed because of gravitational effects. Since surfaces in a natural environment get dirtied after some time, the self-cleaning process is of great importance since they can rid dirt, bacteria, and other environmental contaminants. Two potential mechanisms exist for self-cleaning of natural surfaces: the so-called “lotus effect” and “self-propelled droplets.” In the lotus effect, the surface is cleaned under the action of rain shower. Such leaves have a roughness on the micro- and nano-meter scales. Water droplets in the form of spheres with very little adhesion to the surface as well as dirt particles only contact the tips of these structures. Therefore, contaminating particles roll off quickly under the action of external forces such as gravity or wind flow.

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In places with no precipitation, the dew forms small droplets that merge together spontaneously and are self-propelled automatically off the surface. This requires neither gravity nor wind and provides a fundamentally different self-cleaning mechanism, as recently reported for super-hydrophobic surfaces.⁹ This method of self-cleaning is reported to clean both man-made surfaces⁴ and natural surfaces such as cicada wings, lacewings, and spring-tails.^{1,16,17} The biological importance of this mechanism may be associated with protecting such surfaces from long term exposure to pathogens such as plant fragments, bacteria, and fungi, under conditions where the lotus effect is not possible.

A number of earlier papers have studied droplet jumping induced by droplet coalescence on super-hydrophobic surfaces using experimental, theoretical, and numerical methods. In particular, Boreyko and Chen⁹ reported the first self-propelled jumping experiment of coalescing droplets on a super-hydrophobic surface with radius ranging from 10 μm to 150 μm occurring on engineered surfaces. They showed that the jumping leads to autonomous and rapid removal of the merged droplet. Three stages of coalescence were observed for the super-hydrophobic surface: initial growth without coalescence, immobile coalescence, and mobile coalescence. They measured the vertical velocity of the merged droplet vs. the average diameter of two coalescing droplets experimentally. The results show that the velocity grows with increasing droplet size, reaches a maximum, and then decreases with further increase in size.

Wang *et al.*¹⁸ presented a theoretical analysis based on energy conservation for the self-propulsion during coalescence of droplets over a super-hydrophobic rough surface. Since the scale of droplets in their analysis is much smaller than the capillary length, the gravity force is neglected. The van der Waals interaction energy between two droplets is also neglected, since its magnitude is about six to seven orders less than that of surface energy and the viscous dissipation energy. Their analysis shows that the autonomous vertical motion can only occur for the coalescence of droplets with the radius ranging from several μm to a few millimeters. As a function of the droplet size, they derived a relation for the coalescence-induced velocity of two droplets based on the equilibrium balance of surface energy, kinetic energy, and the viscous dissipation energy, which is consistent with the experimental results of Boreyko and Chen.⁹

Liu *et al.*¹⁹ modeled and studied the mechanism of transformation and jumping of two micro-droplets on surfaces with different degrees of hydrophobicity and roughness. In this work, the driving force and resistance affecting the droplet transformation on three-phase contact line (TPCL) are analyzed and a dynamic equation is proposed based on energy conservation. The solution for a droplet on a flat surface shows that the jumping process will not occur after coalescence which is in agreement with experimental examination of Boreyko.⁹ A wetted droplet on a rough surface either transforms with limited range or stays there without any shape change depending on the roughness of the surface. However, a partially wetted droplet on micro-nano two-tier rough surfaces is shown to be conditionally transformable to Cassie state, and with suitable micro- and nano-structure parameters, jumping can occur upon coalescence. The calculation results also show that for two Cassie state droplets from $O(10)$ micrometer to millimeter scale on textured surfaces, the merged droplet can jump more easily. It is also demonstrated that if the initial size of two droplets is significantly different, the coalescence induced-jumping will not take place.

Peng *et al.*²⁰ simulated the dynamic evolution of two-dimensional droplet size and velocity during droplet coalescence using a multiphase lattice Boltzmann method (LBM) based on the free energy model introduced by Swift *et al.*²¹ They calculated the released surface energy statistically and predicted the jumping height of the merged droplet after coalescence on a super-hydrophobic surface based on the energy conservation method. The results revealed that since the droplet velocity and radius are small, the air friction has little influence on the jumping height of the coalesced droplet.

Nam *et al.*²² presented energy and hydrodynamic analysis with more detailed dynamics during coalescence-induced jumping on super-hydrophobic surfaces using a 3D numerical model. The model is based on the level contour reconstruction method, a scheme which combines the front tracking and level set methods.²³ They validated their numerical results by conducting an experimental study. The dynamic changes in all energy terms during the droplet evolution process including merging and jumping show that approximately 40%–60% of the released surface energy was

converted to kinetic energy at an early stage of the coalescence. At the beginning of the evolution, the neck generated by low pressure is associated with high negative curvature of the liquid bridge which leads to prompt increase in the kinetic energy. As the merged droplet starts detaching from the substrate, the value decreases to approximately 20%–30%. They also showed that the total energy of the entire system is conserved and the predicted droplet jumping velocities were in accord with the measured values.

Liu *et al.*²⁴ simulated the problem of coalescence-induced self-propelled jumping on rough super-hydrophobic surfaces using two-dimensional lattice Boltzmann (LB) method based on the pseudo-potential multiphase LB model proposed by Shan and Chen²⁵ with a real gas equation of state. In order to obtain simulations applicable to high density ratios, the equation of state is modified. The multiple relaxation time (MRT) model²⁶ is also applied to improve the numerical instability issues related to high liquid/vapor viscosity ratios. The jumping velocity and jumping height of droplets with different radii in the simulation were compared with experimental results of Boreyko and Chen.⁹

Liu *et al.*²⁷ carried out a three dimensional numerical study using Navier-Stokes diffuse interface model (NS-DIM) to capture the evolution of air-liquid interfaces where the topology changes rapidly. Their model consists of two identical, static droplets coalescing on a perfectly homogeneous substrate with a contact angle of 180° , without any adhesion, and gravitational effect for droplet radii below the capillary length. Three types of velocities are measured in their simulations: the vertical velocity of the mass center (i.e., droplet velocity), the maximum velocity of the merged droplet, extracted from the evolution of the droplet velocity, and the jumping velocity extracted as a point of transition from strong deceleration to a milder deceleration. This point corresponds to the first pseudo-equilibrium configuration after the departure. The default value of density ratio in their simulation is 50, since a monotonic convergence for the maximum velocity was observed by changing the density ratio from 10 to 100. For the droplet radius larger than the viscous cutoff radius, the capillary-inertial scaling was confirmed by measuring the jumping velocity using both a numerical model and complementary experimental data on textured super-hydrophobic surfaces.⁹ The value of cutoff radius is numerically predicted to be of the order of $0.1 \mu\text{m}$, which is two orders of magnitude lower than the experimental value of $30 \mu\text{m}$. The discrepancy in cutoff radius between numerical and experimental works was suggested to be due to the complex droplet-surface interaction on textured super-hydrophobic surfaces, and the zero adhesion assumption between coalescing droplets and surfaces on flat substrate. The jumping velocity during deceleration of the departed droplet in air is about 0.2 times the capillary-inertial velocity in their simulation, which is in agreement with the experimental value. In the absence of any rotational motion, the kinetic energy of the merged droplet is decomposed into translational and oscillatory components. It was found that a small fraction of the released surface energy is converted into translational kinetic energy for the upward motion, and the energy exchange is mostly between the surface energy and the oscillatory kinetic energy, which eventually is dissipated.

Despite the recent numerical works on the coalescence-induced jumping in the limit of viscous flow, the effect of the ambient environment on the dynamic evolution of droplet has not been studied. The ambient environment may be air of varying humidities or the saturated vapor of the liquid drop itself as in thermal diode applications.²⁸ Although it was shown²⁷ that the inertia of air (i.e., surrounding air density) has no dynamic role prior to jumping of the merged droplet, it has a key role at the later stage of jumping process where the droplet has already jumped into the air. In principle, the gas properties can be varied quite significantly through the pressure and use of mixtures, and the results of the present study illustrate that the density and viscosity of the air affect the jumping process. There is a generation of vortical structure at the stage of jumping, which is weaker for smaller air density, leading to a shorter droplet jumping height at lower air density.

In this paper, we apply a recently proposed LBM^{29,30} to study the evolution of two identical droplets in the coalescence and jumping process, when inertia dominates over viscosity. The method is based on the Cahn-Hilliard diffuse interface theory for binary fluids. This particular free energy-based formulation is preferred in this study because it can eliminate spurious currents at equilibrium and allows larger density and viscosity ratios between the fluid components.^{30–32}

The remainder of the paper is organized as follows. In Sec. II, we briefly review the implementation of the multiphase LBM used in our simulations. Some of the configurations we studied revisit previous work while others are novel. Sec. III presents numerical results for homogeneous surfaces of constant wettability. Finally, the conclusions are reported in Sec. IV.

II. LATTICE BOLTZMANN METHOD FOR BINARY FLUIDS

In the lattice Boltzmann method, one follows the evolution of a density distribution function for fictitious particles moving on a lattice. The velocity is discretized so as to have one lattice spacing per time step, and particle motion consists of one streaming step between neighboring lattice sites followed by a collision step. In this study, we employ the scheme developed by Lee and Liu³⁰ using a scalar order parameter C , which satisfies the convective Cahn-Hilliard equation $\partial_t C + \nabla \cdot (\mathbf{u}C) = \nabla \cdot (M\nabla\mu)$, involving an adjustable mobility parameter M and a chemical potential μ . Two particle distribution functions, g_α and h_α , are used for binary fluids.³⁰ The former is used for the calculation of pressure and momentum of a two-component mixture, and the latter is used as a phase-field function for the transport of order parameter of one component.

The discrete Boltzmann equations for pressure evolution and momentum equations and advective phase-field equation³⁰ are, respectively,

$$\frac{\partial g_\alpha}{\partial t} + \mathbf{e}_\alpha \cdot \nabla g_\alpha = -\frac{1}{\lambda} (g_\alpha - g_\alpha^{eq}) + (\mathbf{e}_\alpha - \mathbf{u}) \cdot [\nabla \rho c_s^2 (\Gamma_\alpha - \Gamma_\alpha(0)) + \mu \nabla C \Gamma_\alpha], \quad (1a)$$

$$\frac{\partial h_\alpha}{\partial t} + \mathbf{e}_\alpha \cdot \nabla h_\alpha = -\frac{1}{\lambda} (h_\alpha - h_\alpha^{eq}) + M \nabla^2 \mu \Gamma_\alpha + (\mathbf{e}_\alpha - \mathbf{u}) \cdot \left[\nabla C - \frac{C}{\rho c_s^2} (\nabla p + C \nabla \mu) \right] \Gamma_\alpha, \quad (1b)$$

where g_α and h_α are the distribution functions corresponding to the discretized velocity $\mathbf{e}_\alpha$, $\mathbf{u}$ is the volume-averaged velocity, c_s is the speed of sound, λ is the relaxation time, and h_α^{eq} , g_α^{eq} are the equilibrium distribution functions given by

$$g_\alpha^{eq} = t_\alpha \left[p + \rho c_s^2 \left(\frac{\mathbf{e}_\alpha \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_\alpha \cdot \mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^2} \right) \right], \quad (2a)$$

$$h_\alpha^{eq} = t_\alpha C \left[1 + \frac{\mathbf{e}_\alpha \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_\alpha \cdot \mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^2} \right], \quad (2b)$$

where t_α is the weight corresponding to $\mathbf{e}_\alpha$, ρ is the mixture density, and p is the pressure. The relaxation time $\tau = \lambda/\delta t$ is related to the kinematic viscosity by $\nu = \tau c_s^2 \delta t$, and Γ_α is given as $\Gamma_\alpha = \Gamma_\alpha(\mathbf{u}) = h_\alpha^{eq}/C$. The macroscopic variables such as C , $\rho\mathbf{u}$, and p are computed from respective moments of the distribution functions h_α and g_α . The composition and the density are related by a linear relation given as $\rho = \rho_d C + \rho_a(1 - C)$, where ρ_d and ρ_a are the bulk densities of two fluids.

The chemical potential in Eq. (1a) is given by the derivative of the free energy with respect to the order parameter. The free energy is given by

$$\Psi = \int_V \left[E_0(C) + \frac{\kappa}{2} |\nabla C|^2 \right] dV + \int_S [\phi_0 - \phi_1 C_s + \phi_2 C_s^2 - \phi_3 C_s^3 + \dots] dS, \quad (3)$$

where V is the system volume and S is the surface area of the substrate. The free energy of the system involves a mixing energy density for binary fluids, where κ is the gradient parameter and $E_0(C) = \beta C^2(C - 1)^2$ is the bulk free energy with constant β , and surface terms which control the solid-liquid interactions with the surface concentration C_s . Proper control of the wetting properties of a fluid on a solid substrate is obtained by formulating the wall free energy polynomial boundary conditions (linear, quadratic, and cubic).^{33,34} In the current paper, the integral of the free energy on solid boundaries employs a cubic boundary condition, where the interactions between the solid and bulk fluids are neglected and only the interactions between the solid and interface are considered. This boundary condition is appropriate for our simulations, when there is a large difference in density between two fluids. This assumption specifies the parameter set: $\phi_0 = \phi_1 = 0$, $\phi_2 = \phi_c/2$, and $\phi_3 = \phi_c/3$, where ϕ_c is a constant to be chosen to recover the desired contact angle at equilibrium. The dimensionless wetting potential $\Omega_c = \phi_c \sqrt{2\kappa\beta}$ is related to the equilibrium contact

angle by $\cos \theta_{eq} = (\sigma_{sg} - \sigma_{sl}) / \sigma_{lg} = -\Omega_c$, where σ_{sg} , σ_{sl} , and σ_{lg} represent the surface tensions of solid/gas, solid/liquid, and liquid/gas, respectively. The proposed boundary conditions were shown to effectively eliminate spurious currents at equilibrium, and the total mass in the system does not change by more than 1% of its initial value.

The equilibrium liquid-vapor interface profile is therefore found when the mixing energy is minimized, with cubic boundary conditions at a solid surface. The interface profile at a plane at equilibrium is then given by $C(z) = [1 + \tanh(2z/D)]/2$, where z is the coordinate normal to the plane interface and D is the interface thickness. Once the surface tension and interface thickness are chosen, β and κ can be specified as $\beta = 12\sigma/D$ and $\kappa = \beta D^2/8$. For detailed discretization of Eqs. (1a) and (1b) boundary conditions, readers are referred to Ref. 30.

III. HOMOGENEOUS SUPER-HYDROPHOBIC SURFACES

In this section, all simulations are started with two initially static droplets, generated at the center of the computational domain for the $D3Q27$ lattice,³⁵ as shown in Fig. 1. These two droplets coalesce on a homogeneous surface with a contact angle of 180° . Thus, the beginning of coalescence is launched when the diffuse interfaces of two droplets overlap at $C = 0.5$. Since the jumping droplets are much smaller than the capillary length, gravity is neglected. Therefore, they can spontaneously jump away from a super-hydrophobic surface due to the release of excess surface energy.

The process of coalescence-induced jumping is described by three independent dimensionless numbers, the Ohnesorge number (Oh), which shows the effect of the viscous and surface energies for two identical droplets, the viscosity ratio (μ_r), and the density ratio (ρ_r), defined as follows:

$$Oh = \frac{\mu_a}{\sqrt{\rho_a \sigma r_0}}, \quad \mu_r = \frac{\mu_d}{\mu_a}, \quad \rho_r = \frac{\rho_d}{\rho_a}, \quad (4)$$

where r_0 is the droplet radius prior to coalescence, μ_d and ρ_d are droplet viscosity and density, and μ_a and ρ_a are the air viscosity and density, respectively. To quantitatively describe the droplet dynamics, the velocity of the merged droplet in this simulation is defined as the y -component velocity of the mass center of the droplet,

$$\bar{v} = \frac{\int_{\Omega} C v_y d\Omega}{\int_{\Omega} C d\Omega}, \quad (5)$$

where Ω is the whole computational domain, y is the vertical direction perpendicular to the substrate, and C localizes the calculation to the droplet. To facilitate a comparison with experimental or numerical work, we normalize all lengths by r_0 . The jumping time and velocity of the merged spherical

FIG. 1. Schematic representation of two droplets coalescence. Each has an initial radius of r_0 and is in a matrix fluid (i.e., air) on a super-hydrophobic surface.

TABLE I. Numerical convergence for various initial droplet radii with $Oh = 0.0375$, $\rho_r = 839$, and $\mu_r = 59$.

r_0 (lattice unit)	12.5	25	50
$v_{max}^* = v_{max}/u_{ci}$	0.266	0.276	0.273

droplets are non-dimensionalized with inertial-capillary time and velocity scaling,⁹ respectively, as

$$\tau_{ci} = \sqrt{\frac{\rho_d r_0^3}{\sigma}}, \quad (6)$$

$$u_{ci} = \sqrt{\frac{\sigma}{\rho_d r_0}}. \quad (7)$$

The velocity scaling has been suggested by balancing the kinetic energy and interfacial stress, when inertia dominates ($Re_{ci} = \sqrt{\rho_d \sigma r_0 / \mu_d^2} \Rightarrow 1$). Grid dependency of the results is tested by comparing the maximum velocity of the merged droplets (v_{max}) determined from the evolution of vertical droplet velocity ($\bar{v}(t)$) of Equation (5), for three different grid resolutions (Table I). The velocity is presented as dimensionless variable with an asterisk in the table. Varying the droplet radius from 12.5 to 50 lattice units results in only a slight change in the maximum velocity. We perform the simulations for the grid resolution with 25 lattice units.

A. Effect of air and liquid viscosity on the jumping process

Figures 2 and 3 illustrate the evolution of two small, identical droplets during coalescence and jumping from a super-hydrophobic surface having a contact angle $\theta = 180^\circ$ with $\mu_r = 58.8$, $\rho_r = 839$ and two Oh numbers, $Oh = 0.0375$ and $Oh = 0.375$. At the beginning of the evolution, a tiny liquid bridge forms between droplets upon coalescence. The bridge then expands rapidly.

For Oh smaller than the critical value 0.1,³⁶ the inertia dominates during coalescence and jumping (Fig. 2). However, as Oh increases toward unity (Fig. 3), the viscous effects dominate during the coalescence and slow down the dynamics, and consequently, there is insufficient energy available for the self-propelled behavior.

According to Ref. 27, the jumping process can be divided into four stages (Fig. 4): (I) formation and growth of a liquid bridge during droplet coalescence; (II) acceleration of the merged droplet on the substrate toward its maximum velocity; (III) removal of the merged droplet from the surface; and (IV) reduction of the upward motion of droplet in the air due to the presence of air friction, and eventually relaxing to a larger spherical shape, after some oscillation.

The jumping velocity is extracted as a point of transition between the strong deceleration in stage III and mild deceleration in stage IV of the merged droplet, where it has left the substrate.²⁷ This point corresponds to the first pseudo-equilibrium configuration after departure. Temporal evolution of the droplet velocity is then shown in Fig. 5 as a function of Oh and compared with those results of diffuse interface method (DIM) in Ref. 27. The value of Oh is varied from 0.0217 to 0.375 corresponding to the variation of droplet and air viscosity, while keeping all other parameters including $\mu_r = 12.9$ and

FIG. 2. Time-lapse images of the simulated coalescence induced jumping on a non-wetting homogeneous surface with $Oh = 0.0375$, $\mu_r = 12.9$, $\rho_r = 50$. The time is scaled by inertial-capillary time scale as $t^* = t/\tau_{ci}$.

FIG. 3. Time-lapse images of coalescence process of two initially static droplets on a non-wetting homogeneous surface with $Oh = 0.375$, $\mu_r = 12.9$, $\rho_r = 50$.

$\rho_r = 50$ fixed. As Oh increases to 0.3, the merged droplet decelerates and departs the substrate with lower rates because of the viscous effect. For $Oh > 0.3$, the merged droplet reaches to a spherical equilibrium shape without jumping away from the substrate.

However, a direct comparison for the maximum velocity of the merged droplet prior to jumping between the two methods (Fig. 6) shows a distinction in the results for $Oh < 0.1$, which is presumably because of diffusion effect (i.e., choice of mobility parameters) in both methods. For more details on the effect of mobility on the jumping process in LBM, readers are referred to Sec. III B. The maximum velocity varies with Oh , which is defined using the liquid viscosity. On the other hand, it does not depend strongly on the air viscosity. However, the jumping velocity v_j at the first pseudo-equilibrium point is a strong function of air viscosity. Fig. 7 demonstrates the effect of the air viscosity on the temporal evolution of velocity by varying the viscosity ratio, and keeping all other parameters including the liquid viscosity and Oh fixed. The results indicate that the air viscosity has a significant effect on detachment of the merged droplet from the substrate. With increasing air viscosity (i.e., decreasing the viscosity ratio μ_r), the circulation within the droplet is suppressed and the merged droplet is inhibited from jumping.

B. Effect of interfacial mobility parameter

The Cahn-Hilliard mobility parameter can control the coalescence dynamics.³⁷ This parameter should be adjusted such that it is large enough to keep the interface near its equilibrium state, but small enough to minimize damping near the interface.³⁸ The relevant dimensionless number that can reflect the interfacial mobility parameter is the so-called S number which is defined as $S = \sqrt{M\mu_d}/r_0$.³⁹ Therefore, the effect of mobility has been studied by changing S from 6.2×10^{-4} to 7×10^{-3} . Fig. 8 demonstrates that when S is increased while all other parameters including Oh are kept constant,

FIG. 4. Time evolution of droplet velocity during the jumping process of Fig. 2.

FIG. 5. Time dependence of instantaneous droplet velocity for various Oh with $\mu_r = 12.9$, $\rho_r = 50$, and $\theta = 180^\circ$. (a) LBM; (b) NS-DIM. The velocity and time are represented as dimensionless variables with an asterisk, $v^* = v(t)/u_{ci}$, $t^* = t/\tau_{ci}$, where u_{ci} is inertia-capillary velocity and τ_{ci} is the inertia-capillary time.

the jumping velocity in stage III is reduced while in stage IV, the departed droplet reaches to its equilibrium shape faster. At early time (stage I), the diffuse interfaces on two droplets touch and coalescence is started. At very early time, larger mobility may lead to faster coalescence. At the point of coalescence (stage II), the interface is unstable and far from the equilibrium. When the mobility is large, instead of having a very sharp cusp shape, the droplet neck gets rounded very quickly. As the merged droplet moves away from the point of coalescence (stage III), the speed of coalescence or neck-radius is determined by the capillary effect. The sharper the curvature, the faster the droplet moves. During stage IV, where the droplet leaves the substrate, at the point of departure, the merged droplet has a cusp-like shape with a point toward the substrate and a rounded shape at the top. In this case if the mobility increases, the point disappears more quickly, and the oscillating droplet reaches to its equilibrium spherical shape faster. For more clarification, the maximum velocity in stage III and the jumping velocity in stage IV of Fig. 8 are provided in Fig. 9. From the results, we notice that varying S from 6.2×10^{-4} to 2.5×10^{-3} in stage III and 1.7×10^{-3} to 7×10^{-3} in stage IV results in a slight change in both maximum and jumping velocities, respectively. Therefore, we decided to select S such that both maximum and jumping velocity results become independent of mobility parameter, and $S = 2.5 \times 10^{-3}$ is the approximate point which satisfies this condition.

FIG. 6. Maximum velocity of the merged droplet prior to jumping as a function of Oh with $\mu_r = 12.9$, $\rho_r = 50$, and $\theta = 180^\circ$. The mobility parameter is about 0.8 in the LBM case.

FIG. 7. Time dependence of vertical droplet velocity with $Oh = 0.0375$, $\rho_r = 800$, and various air viscosities ($\mu_r = \mu_d / \mu_a$).

C. Comparison with experimental data

To validate our results, we compared the jumping velocity at the first pseudo-equilibrium point, with numerical simulation performed by Liu *et al.*,²⁷ and experimental evidence of Boreyko and Chen⁹ with the same fluid properties at 20 °C, except the density ratio in NS-DIM is chosen below 100. The jumping velocity should follow the capillary–inertial scaling $r_0^{-1/2}$. This has been confirmed by the experiments with coalescing droplets of water condensate on textured super-hydrophobic surfaces.⁹ The effect of the coalesced droplet radius on the jumping velocity is presented in Fig. 10. It appears that the two methods are in reasonable agreement with the experiment for larger size droplets. For droplets smaller than 10 μm , the present model is closer to the experimental results than NS-DIM. However, the experimentally measured jumping velocities on super-hydrophobic surfaces are somewhat lower than numerical predictions. There are two sources of discrepancy between the jumping velocity values from numerical simulations and experiments: the first source of discrepancy arises from the fact that both LBM and NS-DIM operate with a zero adhesion assumption between the merged droplet and the substrate. A possible source of the discrepancy especially for droplets smaller than 10 μm on super-hydrophobic surfaces can be explained by an experimentally observation⁴⁰ which

FIG. 8. Effect of mobility on the evolution of the droplet velocity.

FIG. 9. Velocity of the merged droplet as a function of mobility parameter M with $Oh=0.0375$, $\mu_r=12.9$, $\rho_r=50$. ■: maximum droplet velocity prior to jumping in stage III and ▲: jumping velocity in stage IV.

shows a very low contact angle at initial time of droplet growth. Then, the base diameter of droplet increases in a step-like fashion. This stick-and-slip motion can be repeated leading to periodic contact angle oscillations near its maximum value.

It was revealed previously^{9,27} that as long as the droplet radius is above the viscous cutoff, the simulations yield a nearly constant non-dimensional jumping velocity $v_j^* = v_j/u_{ci} = 0.2$, which is confirmed in the current study as well.

D. Effect of air inertia on the maximum and extracted jumping velocities

According to the definition of air Reynolds number ($Re_a = \rho_a u_{ci} r_0 / \mu_a$), at the later stage of jumping, the two variables affecting the air inertia are the air density and dynamic viscosity. Therefore, the air kinematic viscosity ($\nu_a = \mu_a / \rho_a$) influence is studied as a key parameter on the velocity of droplet. Since the dynamic viscosity ratio and, in particular, the air dynamic viscosity are kept constant in this section, changing the air kinematic viscosity reflects the effect of air density. Prior to jumping in stage III, the air density has no dynamic role, which was shown in Ref. 27 for density ratios ranging

FIG. 10. Comparison of numerical simulations of LBM and NS-DIM at 20 °C with the jumping experiment.

FIG. 11. Time dependence of vertical droplet velocity with $Oh = 0.069$, $\mu_r = 60$, and various density ratios.

from 10 to 100. This is confirmed in the current study by comparing the maximum velocity for density ratios varying from 60 to 800 in Fig. 11. However, when the merged droplet departs the surface into the air, the air inertia becomes important in promoting droplet rising. This difference is significant beyond the first pseudo-equilibrium configuration after the departure as depicted in Fig. 11. It can be seen that increasing the air inertia (i.e., decreasing the density ratio) induced larger droplet velocity, raising the droplet higher. To illustrate the effect of air inertia on the structure of flow inside and outside the droplet, analysis of streamlines and vorticity contours is performed before and after jumping. Figures 12–14 show the streamlines on the top panel and the contours of dimensionless magnitude of vorticity on the bottom for three different density ratios. The streamlines have a similar recirculation pattern for all density ratios. As the droplet leaves the substrate into the air, increasing the air inertia (i.e., decreasing the density ratio) results in a development of more vortical structures around the center of droplet. For all density ratios, there is a confluence of these vortical structures along the center of the droplet. Comparing the three air density ratios shows that these vortical structures get weaker as the air inertia is decreased. In terms of vorticity contours, the magnitude of vorticity

FIG. 12. Streamline patterns and absolute value of vorticity contours of flow structure inside and around the merged droplet prior to jumping at $t^* = 2.3$ with $Oh = 0.0375$ and $\mu_r = 60$. (Upper row) Streamlines at three different density ratios and (lower row) absolute value of vorticity contours at three different density ratios. The colors represent vorticity magnitude which is scaled by capillary-inertia time (τ_{ci}). Each column shows streamlines and vorticity contours at the same density ratio.

FIG. 13. Streamline patterns and absolute value of vorticity contours of flow structure inside and around the merged droplet after departure at $t^* = 4.4$ with $Oh = 0.0375$ and $\mu_r = 60$. (Upper row) Streamlines at three different density ratios and (lower row) absolute value of vorticity contours at three different density ratios. The colors represent vorticity magnitude which is scaled by capillary-inertia time (τ_{ci}). Each column shows streamlines and vorticity contours at the same density ratio.

is scaled by capillary-inertia time (τ_{ci}). The contours are generally concentrated in the lighter fluid outside the droplet. In particular, the vorticity tends to migrate to the region of lower density, and this has a key role in the shape of the structure. Prior to jumping, the vortices are formed along the contact line. After droplet departure, the number of vorticity contours is higher for larger air density. These lead to a more highly localized momentum which is diffused less rapidly in the air. As the droplet travels to the equilibrium height (Fig. 14), at larger air inertia, part of the vortices are generated along the droplet interface and part remained near to the substrate. The vorticity magnitude decreases at this height due to viscous dissipation.

An argument based on the surface wettability and Ohnesorge number of the merged droplet allows the construction of a phase diagram. The criterion for a droplet to jump away from the surface can be obtained from the critical Oh (Oh_c) for a fixed contact angle θ and critical value of contact angle on the substrate (θ_c) for a fixed Oh . Fig. 15 presents the phase diagrams of the jumping regimes for a 3D

FIG. 14. Streamline patterns and absolute value of vorticity contours of flow structure inside and around the merged droplet at equilibrium state at $t^* = 17.7$ with $Oh = 0.0375$ and $\mu_r = 60$. (Upper row) Streamlines at three different density ratios and (lower row) absolute value of vorticity contours at three different density ratios. The colors represent vorticity magnitude which is scaled by capillary-inertia time (τ_{ci}). Each column shows streamlines and vorticity contours at the same density ratio.

FIG. 15. Phase diagram for 3D jumping (shaded area with $\triangle$ symbol) with $\mu_r = 60$ and various density ratios.

merged droplet with different values of the density ratio, for $0.02 \leq Oh \leq 0.4$ and $0^\circ \leq \theta \leq 180^\circ$. The critical value of contact angle where the merged droplet jumps away from the substrate is independent of density ratio, $\theta \approx 150^\circ$. Two distinct dynamical regimes for both small and large density ratios can be observed when $\theta \geq 150^\circ$: inertial (shaded area) and viscous regimes. For $\theta < 150^\circ$, the droplet does not depart the surface for any Oh . However, for $\theta > 150^\circ$, Oh_c depends on both density ratio and wettability of the substrate. As the density ratio is increased, Oh_c decreases. At any density ratio, decreasing the wettability of the surface (i.e., increasing θ) promotes the jumping process. Therefore, the critical value of Oh increases and inertia can still play a role in the dynamics.

IV. CONCLUSION

In this paper, we have used a multiphase lattice Boltzmann method to simulate droplet coalescence induced self-propelled jumping on a homogeneous super-hydrophobic surface for a range of Ohnesorge number and density ratio. This paper has mainly focused on the influence of inertia on the jumping height of the droplet. Aside from illustrating the evolving droplet shapes for different Oh , we quantified the behavior in terms of the time dependence of jumping velocity of the merged droplet. As a function of droplet radius, the jumping velocity in both models is compared with experimental evidence of Boreyko and Chen⁹ with the same fluid properties. We find a reasonable agreement between the methods with experiments at larger size droplet. There are two sources of discrepancy: zero adhesion assumption between the merged droplet and the substrate in both models and oscillation of contact angle near its maximum value for smaller size droplet.

To study the effects of both liquid and air viscosity on the evolution of the jumping velocity of the merged droplet, we considered $0.02 \leq Oh \leq 0.4$. The maximum velocity varies with Oh , which is defined using the liquid viscosity, but does not depend strongly on the air viscosity. In this case, as previously studied,²⁷ as Oh increases to 0.3, the merged droplet decelerates and departs the substrate with lower rates. For $Oh > 0.3$, the merged droplet approaches spherical equilibrium shape without jumping away from the substrate. However, the jumping velocity is a strong function of the air viscosity. The results in this case confirmed that the air viscosity effect is significant in detachment of the merged droplet from the substrate. For large air viscosity, the circulation within the droplet is inhibited, and the self-propelled jumping has not been observed.

Aside from observing the viscous effect on the coalescence-induced jumping, there is a need to study the effect of inertia and in particular the air inertia on the dynamic evolution of air-liquid interfaces, since it can have significant effects on the behavior of the merged droplet at the later stage of droplet jumping. The larger the air inertia is the higher the droplet travels against the air. Here, we investigate how inertia affects the structure of flow inside and outside the droplet before and after jumping by analysis of streamline and vorticity patterns. As the merged droplet departs the substrate into the air, increasing the air inertia results in a development of more vortical structures around the

center of the droplet. For all density ratios, there is a confluence of these vortical structures along the center of the droplet. In terms of vorticity, there exists a formation of vortices along the contact line and interface of the merged droplet prior and after jumping. Due to the highly localized momentum around the droplet at higher air density, more vorticity contours are generated after droplet departure.

Finally, we assembled the results in phase diagrams for the lowest and highest density ratios considered here, to obtain the criterion for the jumping of the merged droplet from the critical Oh and critical contact angle. For $\theta < 150^\circ$, the merged droplet does not jump away from the substrate, no matter how large the air density is. However, for $\theta \geq 150^\circ$, there is an Oh_c , below which jumping can occur, depending on both density ratio and surface wettability. As the density ratio is increased, Oh_c decreases, which is due to the effect of air inertia. By decreasing the wettability of the surface, this critical value can be increased such that the inertia can still play a dynamic role.

ACKNOWLEDGMENTS

This work is supported in part by an NSF PREM Grant (No. DMR0934206). This research was also supported, in part, by a grant of computer time from the City University of New York High Performance Computing Center under NSF Grant Nos. CNS-0855217, CNS-0958379, and ACI-1126113.

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