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# Computational study of microparticle effect on self-propelled jumping of droplets from superhydrophobic substrates

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ABSTRACT

We present three-dimensional numerical simulations, employing a lattice Boltzmann method for three-phase system of liquid, gas, and solid, and investigate the influence of a solid particle on the dynamic and departure of a droplet after coalescence on superhydrophobic substrates. A particle can be removed autonomously by the jumping motion of the droplet, which partially or fully covers the particle. This spontaneous removal from superhydrophobic substrates is achieved by converting surface energy to kinetic energy, independent of gravity. We discussed the effect of size, wettability and initial placement of particle on the evolution of lateral and vertical motion of the droplet. The results indicate that the droplet with a fully immersed particle, as in the floating mechanism, reaches to the same equilibrium height as a particle-free droplet. However, the droplet with a partially immersed particle, as in the lifting mechanism, can have a substantial jumping velocity compared to a particle-free droplet. As the size of the partially immersed particle approaches its critical limit, which is equal to the size of the droplet, the droplet jumping and transport from the substrate is enhanced. Besides the particle size, the particle wettability can result in a considerable droplet jumping velocity. A particle with a neutrally wetting contact angle (i.e. 90°) is found to elevate the transport of the droplet to a higher distance from the substrate relative to a partially wetting case (i.e. 60°). In the lifting removal mechanism, unlike the floating removal mechanism, the particle initial placement is highly critical for the detachment of the merged droplet from the substrate, as well as the elevation of the detached droplet to a longer distance from the substrate. For a partially immersed particle, the critical particle initial position from the substrate above which the droplet-particle system does not jump away from the substrate is independent of particle size and wettability and is about $1.5r_d$ where $r_d$ is the initial size of the droplet.

## 1. Introduction

The coalescence-induced jumping of a microdroplet from superhydrophobic substrates has attracted much attention for various biological and industrial applications, including self-cleaning surface applications (Wisdom et al., 2013), condensation heat transfer enhancement (Cheng et al., 2012; Dietz et al., 2010; Miljkovic et al., 2013a; Torresin et al., 2013), anti-icing (Boreyko and Collier, 2013; Cao et al., 2009; Zhang et al., 2013), anti-dew (Boreyko and Chen, 2009; Feng et al., 2012; Rykaczewski et al., 2012b), and anti-corrosion (Narhe et al., 2010). This spontaneous removal from structured superhydrophobic substrates offers an alternative way for the self-cleaning process under humid conditions, as was reported first by Boreyko and Chen (2009). The micro- and nano-structures of natural surfaces such as cicada wing (Wisdom et al., 2013) or gecko skin (Watson et al., 2015) help the dew droplet to coalesce and become bigger. Then the merged droplet self-propels itself and jumps perpendicular to the substrate, due to the sudden release of the surface energy. This process requires neither gravity nor wind and provides a fundamentally different self-cleaning mechanism than the conventional lotus effect (Wisdom et al., 2013). The self-propelled jumping has not been observed for droplet sizes comparable to or larger than the capillary length (Menchaca-Rocha et al., 2001; Mertaniemi et al., 2012; Nilsson and Rothstein, 2011), where the gravitational force becomes effective. Furthermore, such non-wetting substrates presenting self-propelled jumping of droplet were shown not to be sensitive to the contact angle hysteresis (less than 5%) (Miljkovic et al., 2013b), which is due to the spontaneous removal of the merged droplet at length scales well below the capillary length.

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The main advantage of this new removal mechanism is that it can act effectively at any orientation with no external force. Owing to their extremely small size, the self-propelled droplets can travel further to a sufficient distance beyond the boundary layer of the substrate using a slight breeze or surface-parallel shear flow. If the substrate is oriented horizontally, the merged droplet may eventually return to the substrate and trigger more droplets to lift off, as long as the size of the returned droplets are smaller than the capillary length. The biological importance of this new removal mechanism is associated with protecting natural surfaces from long term exposure to pathogens such as plant fragments, bacteria and fungi, under conditions where rainfall is absent for long periods of time and the lotus effect is not possible (Watson et al., 2015; Wisdom et al., 2013). This jumping motion can therefore explain an easy and rapid global transport of dirt, bacteria and other contaminating particles from the surface, which promises remarkable savings in energy and natural resources.

Despite the recognized importance of the particle removal, only one experimental study can be found in the literature that discusses the macroscopic behavior of coalescence-induced self-propulsion of droplets for the transport of such particle. Wisdom et al. (2013) revealed autonomous removal of both hydrophobic/hydrophilic and organic/inorganic particles with different wettabilities and sizes. The self-propelled removal mechanism is shown to be more effective for particles with a diameter as large as 100µm. The self-cleaning process of particles in their study was demonstrated for particles greater than 8µm in diameter, because of difficulty of high-speed imaging. Three different processes of particles removal were recognized, depending on their wettability: floating, lifting, and aggregating. In the floating removal mechanism with very hydrophilic particles, the results revealed that the particles have a tendency to detach into the bulk fluid from the air-liquid interface. However, the lifting mechanism occurs when less hydrophilic particles are partially covered with the liquid droplet. Although the capillary-inertial processes lead to the jumping droplet, the experimental results revealed a major difference in both floating and lifting removal processes of particles from superhydrophobic substrates. In the floating removal mechanism, the particle is removed from the substrate before the merged droplet jumps away from the substrate, whereas, in the lifting removal mechanism the particle is lifted away from the substrate by the merged droplet after its jumping motion.

Studies on the influence of parameters involved in contaminating particle removal upon coalescence-induced self-propelled jumping of droplets from superhydrophobic substrates are still lacking. The properties of the particle, e.g., wettability and size, and the surrounding fluid, allow particle and droplet to travel through either atmospheric or ambient environments for a relatively long time and distance. Furthermore, depending on the particle wettability and initial position, inclusion of a single particle can lead to the surface-parallel departure of the droplet from the boundary layer of the substrate without need of a surface-parallel shear flow. These phenomena have not been investigated from the simulation point of view, to authors' best knowledge. A number of earlier papers have studied the particle-free droplet jumping induced by droplet coalescence on superhydrophobic substrates using numerical methods. Nam et al. (2013) presented energy and hydrodynamic analysis during coalescence-induced jumping on superhydrophobic substrates using a three dimensional numerical model, which combines the front tracking and level set methods. Peng et al. (2013) simulated the dynamic evolution of two dimensional droplet during coalescence using a multiphase lattice Boltzmann method (LBM) based on the free energy model. Liu and Cheng (2015) adopted three dimensional LBM based on the pseudo-potential multiphase LBM, to study morphological effects on the self-propelled jumping of droplet on rough superhydrophobic substrates. Liu et al. (2014) conducted the three dimensional study using Navier–Stokes diffuse interface model (NS-DIM) to capture the evolution of air-liquid interfaces where the topology changes rapidly. Shi et al. (2015) simulated coalescence-induced droplet jumping behavior on superhydrophobic complex textured substrates using three-dimensional multi-relaxation-time pseudo-potential LBM. Farokhirad et al. (2015) performed lattice Boltzmann (LB) simulations to investigate effects of air inertia and viscosity on the evolution of the droplet jumping. With three dimensional NS-DIM, Cheng et al. (2016) studied effect of droplet size and contact angle hysteresis on the jumping process.

In this paper, we apply a recently proposed LBM technique (Connington et al., 2015) to simulate the self-propelled jumping of droplets containing a single particle. The proposed method combines the multi-component (Lee, 2009; Lee and Liu, 2010) and particle dynamics algorithms that are capable of eliminating spurious currents at equilibrium, thus can employ components with sufficiently large density differences (Farokhirad et al., 2013; 2015; Zhang et al., 2014). The remainder of the paper is organized as follows. In Section 2, the numerical method used in our simulations is briefly reviewed. A few configurations studied revisit the previous work while others are novel. Results of the numerical simulations are discussed in Section 3. Our findings would shed insights on the development of a rapid self-cleaning mechanism, which may be difficult to investigate experimentally. Finally, the conclusions are reported in Section 4.

## 2. Lattice Boltzmann method for binary fluids

We implement the LBM proposed by Lee and Liu (2010), based on the Cahn–Hilliard diffuse interface theory for binary immiscible fluids. In this theory, an interface between binary fluids evolves so that the total free energy of the system is minimized. The total free energy contains both local and nonlocal terms, as well as contributions from solid boundaries and is written as:

$$\Psi = \int_V \left[ E_0(C) + \frac{\kappa}{2}|\nabla C|^2 \right] dV + \int_S \left[ \phi_0 - \phi_1 C_s + \phi_2 C_s^2 - \phi_3 C_s^3 + \ldots \right] dS, \tag{1}$$

where $V$ is the volume of the system and $S$ is the surface area of the substrate and the solid particle. The local part of the bulk free energy, namely the mixing energy, is $E_0(C) = \beta C^2 (C-1)^2$, where $\beta$ is the bulk free energy constant, and $C$ is the composition or the order parameter. The gradient coefficient $\kappa$ in the nonlocal term controls the surface tension and interfacial thickness. In the surface integral, $C_s$ denotes the composition at the solid surface and the $\phi_i$'s are constant coefficients. The out of equilibrium binary system advances toward its minimal energy state according to the Cahn–Hilliard equation:

$$\partial_t C + \nabla \cdot (\mathbf{u} C) = \nabla (M \nabla \mu), \tag{2}$$

where $\mathbf{u}$ is the volume-averaged mixture velocity, $M$ is the mobility parameter, and µ is the chemical potential extracted from the total free energy upon variation, and is written as $\mu = \mu_0 - \kappa \nabla^2 C$, with $\mu_0 = \partial E_0 / \partial C$ being the classical (local) part. The solution to Eq. (2) requires two boundary conditions. The boundary condition for $\nabla^2$µ ensures no mass flux due to the nonzero chemical potential gradient in the direction normal to the solid surface ($\mathbf{n} \cdot \nabla \mu|_s = 0$), where $\mathbf{n}$ is the normal unit vector to the surface. The boundary condition for $\nabla^2 C$, is established by minimizing the surface free energy subject to the specified wall free energy (Lee and Liu, 2008; Liu and Lee, 2009). We use the cubic boundary condition which specifies the parameter set $\phi_0 = \phi_1 = 0$, $\phi_2 = \phi_c/2$, and $\phi_3 = \phi_c/3$, where $\phi_c$ is chosen to recover the desired contact angle at equilibrium. The boundary condition for $\nabla^2 C$ therefore becomes $\mathbf{n} \cdot \nabla C|_s = \frac{\phi_c}{\kappa}\left(C_s - C_s^2\right)$. A planar interface profile at