Directional migration of an impinging droplet on a surface with wettability difference

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On designed heterogeneous surfaces, the lateral motion of a droplet can be controlled without requiring an external energy input. However, it is still a challenge to elaborately manipulate the self-migration behaviors of an impinging droplet because of a lack of fundamental understanding of these behaviors. Through direct numerical simulation, a wide range of parametric studies are conducted to investigate the effect of the Weber number (We), wettability difference, and offset impinging on the four phases—symmetric spreading, directional retracting, detaching, and migrating—of droplets impacting heterogeneous surfaces. The results indicate that asymmetric spreading and directional retracting toward the hydrophilic area are induced by the unbalanced net forces acting on the three-phase contact line. The increase in the wettability difference leads to the increase in the migration distance from the borderline, the decrease in the droplet bouncing height, and the decrease in the contact time between the liquid and the nonwetting area. An increasing We influences the spreading diameter and the migration distance, but no significant difference can be observed during the retracting and detaching stages for moderate We owing to the combined effect of the spreading rate and the surface tension force. In addition, offset impinging plays a major role in droplet spreading and deformation. These physical insights provide developing guidelines for the design of surfaces to manipulate the behaviors of impinging droplets.

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I. INTRODUCTION

Controlling liquid droplet motion is a challenge but an essential technology for areas ranging from self-cleaning to water harvesting. Among the proposed strategies, such as electrowetting [1,2], the Leidenfrost effect [3,4], substrate vibration [5,6], or surface charge [7], proper design of the wettability gradient by chemical heterogeneity or structural topography has been demonstrated to be an effective way to manipulate droplet transportation on solids [8].

This mechanism was identified by Greenspan [8], and analyzed by Greenspan [8] and Brochard [9], followed by some experimental demonstrations [10–13]. They found that the self-motion of the droplet on gradient surfaces results from the imbalance of forces acting on the three-phase contact line (TPCL) around the drop periphery [13–15], pointing toward the direction of increasing wettability, or decreasing contact angle, which is given by $dF_Y = \sigma(\cos \theta_A - \cos \theta_B)dx$, where F_Y is the unbalanced Young's force experienced by the droplet [9], σ is the surface tension coefficient of the liquid-air interface, θ_A and θ_B represent the local contact angles at two different surfaces, and dx is the length of the contact line. Chaudhury [10] experimentally demonstrated the uphill motion of a water droplet induced entirely by the surface chemical gradient on an inclined substrate (15° from

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the horizontal plane). Daniel and Chaudhury [11] found that drops moved with enhanced speeds of 5–10 mm/s upon application of the periodic imbalance force.

Inspired by those early investigations, several droplet controllable surfaces have been fabricated to date by employing structural topography, chemical strips, or hydrophobic or hydrophilic decorations [16]. For instance, Liu [17] designed a gradient surface by gradually increasing the fraction of physical patterns and nanopillars such that the equilibrium contact angle (ECA) θ_e changed from 166.0° to 15.5°, thus achieving directional and long-range transportation of the droplet. Seo [18] proposed that droplet moving, merging, and mixing could be precisely controlled by adjusting the density of the micropillars. Bliznyuk [19,20] studied strip-patterned surfaces and observed the scaling behavior of contact angles, parallel spreading to the stripes, and motion restriction to the perpendicular direction in response to the varying stripe widths. Deng [21] decorated the high-adhesion substrates with a special wedge pattern and achieved directional motion of the droplet. In addition, droplet behavior can be projected, and the transport distances can also be controlled by adjusting the wedge angle and the droplet size. More recently, Chai [22] found that the synergy between the structural gradient, chemical gradient, and wrinkled structure caused the droplet to undergo unidirectional spreading, and dynamic regulation of the spreading length on the flexible structure was achieved.

Although the surfaces in these studies manipulate the lateral migration of a droplet from the steady state well, the investigative requirement of droplet impinging on the designed surface should be satisfied because droplets in industries always involve impacting, spreading, and rebounding behaviors, which depend on the following parameters: wettability, impact velocity, viscosity, and surface tension [23]. More recently, some studies involving water droplet impinging on gradient surfaces have been conducted. For example, Malouin [24] investigated the axial rebound of the droplet and proposed that the placement and trajectory of impinging droplets could be controlled by engineering nonuniform textures on the substrate. Li [25] experimentally and numerically demonstrated the gyrating and bouncing behavior of droplets impacting hydrophobic surfaces decorated with hydrophilic strips. In addition, the droplet was observed to split when it impinged at a high velocity on a hydrophilic surface with a single hydrophobic strip [26]. To the best of our knowledge, most of these studies focused on exploring the novel bouncing and migrating behaviors of the droplet, whereas only two experiments [27,28], investigated the fundamental effect of the wettability difference and impact velocity on the droplet behavior. In the experiments described in Refs. [27,28], the offset impinging of a droplet on a substrate with wettability difference $\Delta\theta_e = \theta_{\text{pho}} - \theta_{\text{phi}}$, where θ_{pho} and θ_{phi} represent the ECA for the hydrophobic and hydrophilic areas, respectively, was investigated. However, their study on the offset impinging, the limited wettability difference, and the Weber number effect $We = \rho D_0 u^2 / \sigma$ is insufficient to fully understand droplet impinging behaviors on heterogeneous substrates, where ρ represents the density, D_0 is the droplet diameter, and u is the velocity.

To gain a full understanding of the problem and obtain physical insights, three-dimensional direct numerical simulation (DNS) is employed in the present study, which is based on the coupled level-set and volume of fluid (CLSVOF) method [29–35] for the interface tracking, avoiding the individual drawbacks of the VOF and the level-set method. It was demonstrated in our previous studies [35,36] that the simulation results matched the experimental results well for the complex two-phase flow [35] and the droplet wall interaction [36]. When the liquid meets the solid, however, the drop shape and behavior are critically determined by the surface property. For example, the impacting droplet exhibits the pancake bouncing phenomenon on superhydrophobic (super nonwetting) surfaces [37], whereas the liquid spreads completely and then forms a flat film rather than a droplet on superhydrophilic (superwetting) substrates [38]. Therefore, the apparent contact angle θ_{app} should be inserted into the boundary condition to consider the effect of the surface property on liquid behaviors [31]. Here, the mesh-dependent contact angle model [39] is employed, and the contact angle implementation scheme is based on the functions developed by Sussman [40] because of its simplicity: there is no need to locate the position of the TPCL.

The objective of this study is to numerically investigate the effects of the Weber number We , wettability difference $\Delta\theta_e$, and offset impinging on the asymmetric spreading, directional rebounding, detaching, and migrating behaviors of a droplet impinging on a surface with a wettability difference. The paper is organized as follows. The numerical method and physical problem modeling are presented in Sec. II. In Sec. III, the numerical method is validated against the data from Ref. [41]. The detailed results are discussed in Sec. IV, and concluding remarks are presented in Sec. V.

II. METHODS AND MODELING

A. DNS

A droplet consists of Newtonian and incompressible liquid, with no phase change during the impingement. Interfacial forces originate from the curvature only. At the TPCL, a dynamic contact angle is implemented. Based on these assumptions, the continuity and momentum equations applied to DNS using the in-house code FK³ [35,36] can be expressed as

$$\nabla \cdot \mathbf{u} = 0, \quad (1)$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla P + \nabla \cdot \mu [\nabla \mathbf{u} + (\nabla \mathbf{u})^T] + \rho \mathbf{g} + \mathbf{F}_\sigma, \quad (2)$$

where P , μ , and ρ are the pressure, viscosity, and density, respectively, and $\mathbf{g}$ is the acceleration due to gravity.

The density ρ and viscosity μ in Eq. (2) are smoothed by the Heaviside function $H_\Gamma(\varphi)$ and are defined as

$$\rho = \rho_l H_\Gamma(\varphi) + \rho_a [1 - H_\Gamma(\varphi)], \quad (3)$$

$$\mu = \mu_l H_\Gamma(\varphi) + \mu_a [1 - H_\Gamma(\varphi)], \quad (4)$$

$$H_\Gamma(\varphi) = \begin{cases} 0 & (\varphi < -\Gamma) \\ \frac{1}{2} \left[1 + \frac{\varphi}{\Gamma} + \frac{1}{\pi} \sin \left(\frac{\pi \varphi}{\Gamma} \right) \right] & (|\varphi| \leq \Gamma) \\ 1 & (\varphi > \Gamma) \end{cases} \quad (5)$$

where a and l represent the air and liquid, respectively, φ is the level-set function, Γ represents the half-thickness of the air-liquid interface, which is typically chosen as one or two grid distances. We use $\Gamma = 1.5\Delta$, where Δ is the mesh size.

$\mathbf{F}_\sigma$ in Eq. (2) denotes the momentum source term concerned with the surface tension force, which is calculated using the continuum surface force (CSF) method proposed by Brackbill [42]:

$$\mathbf{F}_\sigma = \sigma \kappa \mathbf{n}_\varphi \delta_\Gamma(\varphi), \quad (6)$$

where κ , $\mathbf{n}_\varphi$ are the curvature and the normal vector of the interface given by

$$\kappa = -(\nabla \cdot \mathbf{n}_\varphi) = -\frac{1}{|\nabla \varphi|} \left[\frac{\nabla \varphi}{|\nabla \varphi|} \cdot \nabla |\nabla \varphi| - \nabla \cdot \nabla \varphi \right], \quad (7)$$

$$\mathbf{n}_\varphi = \frac{\nabla \varphi}{|\nabla \varphi|}, \quad (8)$$

and $\delta_\Gamma(\varphi)$ denotes the delta function [32] used to limit the effect of the surface tension and improve the stability of the standard CSF model in a narrow region at the interface:

$$\delta_\Gamma(\varphi) = \begin{cases} 0 & (|\varphi| > \Gamma) \\ \frac{1}{2\Gamma} \left[1 + \cos \left(\frac{\pi \varphi}{\Gamma} \right) \right] \left[1 + \frac{\varphi}{\Gamma} + \frac{1}{\pi} \sin \left(\frac{\pi \varphi}{\Gamma} \right) \right] & (|\varphi| \leq \Gamma) \end{cases} \quad (9)$$

B. Interface-capturing scheme

For the CLSVOF method [35], the level-set function is employed to compute the curvature and the normal vector to the interface accurately, and the VOF function is utilized to reconstruct the interface. Therefore, from Eqs. (3)–(9), φ represents the level-set function defined at each calculation grid center that is positive in the liquid and negative in air. The initial value $\varphi_{i,j,k}^0$ is defined based on the volume fraction $0 \leq C_{i,j,k}^0 \leq 1$ to identify each phase separately:

$$\varphi_{i,j,k}^n = (C_{i,j,k}^n - C_{int})\Gamma, \quad (10)$$

where $C_{int} = 0.5$ denotes the VOF value on the interface, and n represents the time step.

In the VOF method, the interface-capturing advection equation is simplified using the continuity equation:

$$\frac{\partial C_{i,j,k}}{\partial t} + \nabla \cdot (C_{i,j,k} \mathbf{u}_{i,j,k}) - C_{i,j,k} \nabla \cdot \mathbf{u}_{i,j,k} = 0. \quad (11)$$

The $C_{i,j,k}$ evolved using the weighted linear interface calculation method (WLIC) in Eq. (11) is discretized with the fractional step method [31–33].

To obtain a valid signed-distance function $\varphi_{i,j,k}^{n+1}$, a reinitialization must be considered, and the one we employ in our implementation is due to Ref. [34].

Although the level-set function can be computed with Eq. (10), its transport via $\varphi_t + \mathbf{u} \cdot \nabla \varphi = 0$ will destroy the signed-distance property, and thus the transported level-set function cannot be utilized for the approximation of the surface curvature, normal vector, and surface tension. Hence, a reinitialization process is necessary to obtain a valid signed distance. In the calculation, we evolve $\varphi_{i,j,k}^n$ according to the following Hamilton–Jacobi equation:

$$\frac{\partial \varphi_{i,j,k}^n}{\partial \tau} + S(\varphi_{0,i,j,k}^n) \frac{\nabla \varphi_{0,i,j,k}^n}{|\nabla \varphi_{i,j,k}^n|} \cdot \nabla \varphi_{i,j,k}^n = S(\varphi_{0,i,j,k}^n), \quad (12)$$

where $S(\varphi_{0,i,j,k}^n) = \frac{\varphi_{0,i,j,k}^n}{\sqrt{\varphi_{0,i,j,k}^{n2} + \Gamma^2}}$ is a sign function, $\varphi_{0,i,j,k}^n = \varphi_{i,j,k}^n|_{\tau=0}$, τ denotes the artificial time step, and the secondary accuracy essentially nonoscillatory (ENO) scheme is used for the discretization of Eq. (12). In addition, the convective terms should satisfy the Courant–Friedrichs–Lewy (CFL) condition [34]. We dynamically control the time step τ to enforce the stability limits imposed by the Courant number and capillary time scales, and the initial dimensionless Courant number $C_{fl} = u\tau/\Delta$ is chosen as 0.2 in our simulations.

C. Contact angle boundary condition

At the TPCL, the contact angle is implemented using the method developed by Sussman [40], which is a simple and straightforward scheme even for three-dimensional cases because we do not need to locate the position of the TPCL, and the ghost value of the level set is extrapolated by the advection of the level-set function into the solid based on the contact angle. Its effectiveness has been proved by various studies [31,32]. In the present study, the contact angle boundary condition developed by Voinov [39] is employed:

$$\theta_{\text{num}}^3 = \begin{cases} \theta_{\text{app}}^3 - 9Ca \ln\left(\frac{K}{\Delta/2}\right) & (0 \leq \theta_{\text{app}} \leq \frac{3\pi}{4}) \\ (\pi - \theta_{\text{app}})^3 + 2.25\pi \ln\left(\frac{1 - \cos(\theta_{\text{app}})}{1 + \cos(\theta_{\text{app}})}\right) - 9Ca \ln\left(\frac{K}{\Delta/2}\right) & (\frac{3\pi}{4} < \theta_{\text{app}} \leq \pi) \end{cases}, \quad (13)$$

where θ_{num} is the mesh- and velocity-dependent geometric boundary condition required for solution of the macroscopic hydrodynamic equations, θ_{app} is the apparent contact angle in the macroscopic region that can be obtained with existing empirical functions such as Kistler’s law [43]—Eq. (14)—which is a function of the capillary number $Ca = \frac{\mu u_{cl}}{\sigma}$ and θ_e , where u_{cl} is the contact line velocity [36]. K represents the macroscopic length scale given by the capillary length $K = \sqrt{\sigma/\rho g}$. $\Delta/2$

FIG. 1. Schematic of the computational domain and conditions.

denotes where the slip occurs due to the staggered grid utilized in this study. A detailed description can be found in our previous study [36]. Hence, a much coarser mesh scheme can provide realistic results,

$$\theta_{\text{app}} = f_H[\text{Ca} + f_H^{-1}(\theta_e)], \quad (14)$$

$$f_H(x) = \arccos \left\{ 1 - 2 \tanh \left[5.16 \left(\frac{x}{1 + 1.31x^{0.99}} \right)^{0.706} \right] \right\}. \quad (15)$$

D. Modeling of the problem

A schematic of the computational domain with a uniform, staggered $320 \times 300 \times 320$ grid extending five times as large as the drop diameter $D_0 = 2$ mm is shown in Fig. 1. The droplet (in red) is released at a lateral offset with respect to the borderline, where the left hydrophobic region (in dark gray) meets the right hydrophilic area (in pale gray). Here, we define that the offset is negative, zero, or positive if the droplet impact center is in the hydrophobic area, on the borderline, or in the hydrophilic region, respectively. The distance between the wall and the droplet center is set as $0.55 D_0$ to allow the droplet to develop in a physical manner before touching the solid. Although different definitions of surface wettability can be found, here the adopted wetting and nonwetting surfaces are based on the classification by Iglaier [44]. Accordingly, the hydrophilic area is fixed as the surface of “weakly water-wet” $\theta_{\text{phi}} = 60^\circ$ or “strongly water-wet” $\theta_{\text{phi}} = 30^\circ$, while various wettability surfaces ranging from “neutrally wet” to “strongly nonwetting” are introduced in the hydrophobic region, and hence the wettability difference $\Delta\theta_e$ ranges from 30° to 120° . The utilized hydrophobic and hydrophilic surfaces are shown in Table I. In addition, we limit the study to the

TABLE I. Contact angles of the adopted hydrophobic and hydrophilic surfaces based on the classification of surface wettability by Iglaier [44].

$\Delta\theta_e$ (deg)	θ_{pho} (deg)	θ_{phi} (deg)
30	90	60
60	120	60
90	150	60
120	150	30

FIG. 2. Droplet shape comparison between the present simulation (in red) and experiment [41] (in black) for the droplet impact strongly water-wet surface $\theta_e = 50^\circ$ (a), neutrally wet surface $\theta_e = 90^\circ$ (b), and completely nonwetting surface $\theta_e = 180^\circ$ (c); droplet diameter $D_0 = 2.28$ mm and impact velocity $u_0 = 0.35$ m/s, corresponding to $We = 3.84$.

no-splashing regime by imposing $We \leq 30$ [45], based on which the initial impact velocity u_0 is set in each impact simulation. In addition, the boundary condition of the substrate is set as the wall, while the surroundings are considered as an open space under the free-slip condition. In all cases, the gravitational force $g = 9.8$ m/s² is imposed. The density ratio and viscosity ratio between the liquid and air are constant at $\rho_l/\rho_a = 1000/30$ and $\mu_l/\mu_a = 55$, in which a high air density (under about 2.5 Mpa) is utilized in our simulation to enhance numerical stability. Note that the effects of the viscosity and density ratios decrease rapidly and become insignificant when $\rho_l/\rho_a \geq 10$ [46,47]. In addition, according to the existing mathematical equations [48], the droplet spreading factor is related to the Reynolds number Re , Weber number We , and contact angle, while the liquid-wall contact time [49] is expected to be a function of D_0 , ρ_l , and σ . Therefore, the density ratio ($\rho_l/\rho_a > 30$) utilized in the present study is acceptable.

III. NUMERICAL VALIDATION

To validate the numerical models, we first conduct three simulations of a water droplet impact on homogeneous surfaces with different wettabilities $\theta_e = 50^\circ$, 90° , and 180° , and then compare the results with those from the previous experiment [41]. Except for the density ratio, other impact conditions such as the droplet diameter and impact velocity match the experiment well. The snapshot comparison in Fig. 2 illustrates good agreement on droplet shape evolution between the simulations and the experiments. Next we conduct another series of simulations to make comparison of the spreading factor β in Fig. 3, defined as the ratio of the surface spreading diameter D to the initial droplet diameter D_0 , $\beta = D/D_0$, which reaches the maximum spreading factor β_m when the droplet enters its maximum spreading stage. Figure 4 compares the apparent contact angle measured by the experiment and that predicted by the present simulation. These comparisons show that although there are some differences in narrow regions, the simulations capture the primary features of droplet deformation on solid surfaces well. Therefore, the present numerical method can be used to investigate the dynamics of the impacting droplet on a substrate with a wettability difference.

Finally, three more cases with different grid sizes are employed to examine the grid independence by comparing the maximum spreading factor β_m and the relative error with respect to the experiment. In all simulations, the droplet with diameter $D_0 = 2.1$ mm and velocity $u_0 = 0.5$ m/s impacts the neutrally wet surface $\theta_e = 90^\circ$. Based on the grid independence test in Table II, the grid size is set to $32 \mu\text{m}$ for the simulations performed hereafter in this study.

FIG. 3. The time evolution of spreading factor β for droplet impinging different surfaces, droplet diameter $D_0 = 2.1$ mm and impact velocity $u_0 = 0.5$ m/s, corresponding to $We = 7.21$ [41].

FIG. 4. The time evolution of apparent contact angle for droplet impinging different surfaces, droplet diameter $D_0 = 2.1$ mm and impact velocity $u_0 = 0.5$ m/s, corresponding to $We = 7.2$ [41].

TABLE II. Grid independence test for the three different grid sizes.

Grid size	$\Delta = 50 \mu\text{m}$	$\Delta = 32 \mu\text{m}$	$\Delta = 25 \mu\text{m}$
β_m	1.610	1.628	1.632
Relative error	3.07%	1.95%	1.74%

IV. RESULTS AND DISCUSSION

Simulations are first conducted to examine the effect of the wettability difference, after which the detailed physical insights into asymmetric spreading and directional rebounding are presented. Subsequently, Weber number influences are discussed. Finally, three cases are investigated to understand how the offset affects the droplet impact dynamics.

A. Wettability difference effect

When the droplet impinges the homogeneous substrate, the evolution can be described by four phases: the kinematic phase, spreading phase, relaxation phase, and wetting or equilibrium phase [50]. Here, in the present study, on a surface with a wettability difference, four new phases—the asymmetric spreading phase, retracting phase, detaching phase, and migrating phase—are defined based on the simulation results.

The selected images in Fig. 5 show the evolution of the impinging drop on substrates with four different wettability differences of 30° , 60° , 90° , and 120° at a constant $We = 10$, where the four new phases are observed. For all cases from 2.0 to 3.2 ms, asymmetric spreading governed by inertia is demonstrated due to the wetting difference between the two sides of the borderline. The surface tension and viscosity of the fluid act together against drop spreading until the motion of the contact line terminates, leading to the maximum spreading stage, after which the liquid in the left hydrophobic area directionally retracts and rebounds toward the hydrophilic area. The so-called retracting phase occurs owing to the surface tension effect, which minimizes the free surface of the drop. Subsequently, the detaching phase begins at approximately 9.6 ms when the droplet completely leaves the hydrophobic area, followed by another phase during which the droplet directionally migrates to the more wettable region.

FIG. 5. Time evolution of impinging water droplet on the substrate with varying wettability difference $\Delta\theta_e$ at 30° , 60° , 90° , and 120° for the fixed offset = 0.0, $We = 10$, corresponding to $u_0 = 0.60 \text{ m/s}$.

FIG. 6. Schematic illustration of the droplet body deformation at retracting stage on the homogeneous surface (in solid blue) and on the surface with wettability difference $\Delta\theta_e = 60^\circ$ (in solid red). The black dashed line represents the borderline in Fig. 1, the curve dashed lines represent the surface tension force profile along the TPCL, and the arrows represent some surface tension forces acting at the TPCL.

For a small wettability difference at 30° , partial bouncing [51] of the droplet from the surface is illustrated (see Video S1 of the Supplemental Material [52]) and the corresponding physical insight is discussed subsequently. This directional rebound behavior (called oblique rebound in [53]) was also observed by Reyssat *et al.* [53], where the oblique rebound behavior was more obvious for droplets impinging strong nonwetting surfaces with roughness gradient. Other than the oblique rebound, some other deformation behaviors of droplets such as directional migration and splitting by borderline can be observed subsequently in this work. For cases with moderate $\Delta\theta_e$ values of 60° (see Video S2 of the Supplemental Material [52]) and 90° , droplets migrate only directionally on the surface toward the hydrophilic area without leaving the surface. As the wettability difference increases to 120° (see Video S3 of the Supplemental Material [52]), a large amount of liquid moves toward and adheres to the hydrophilic area, leading to rapid detaching from the superhydrophobic region. In addition, from the droplet state at 15.6 ms, it can be concluded that the increase in the wettability difference increases the migration distance with respect to the borderline, and decreases the droplet bouncing height.

The schematic in Fig. 6 compares the TPCL and droplet appearance at the retracting stage on the homogeneous (in solid blue) and heterogeneous (in solid red) surfaces. It can be observed that the net surface tension force in the lateral direction is zero for the droplet on the homogeneous surface, whereas it points to the x -positive direction on the surface with a wettability difference. According to Ref. [21], the substrate property of the contact angle is crucial in the determination of the net force obtained by integrating the surface tension force in the x component along the contact line. Therefore, an unbalanced net force is generated owing to the wettability difference, driving the droplet to asymmetric spreading and directional migration toward the more wetting area.

The sectional view in Fig. 7 shows clues regarding the asymmetric spreading, retracting, and directional migrating behaviors of a droplet. At 3.8 ms, the central liquid spreads nonuniformly due

FIG. 7. Sectional views of the velocity field illustrating the droplet asymmetric spreading, retracting, and directional migrating mechanism on the surface with $\Delta\theta_e = 60^\circ$, and $We = 10$. Snapshots and arrows are colored by the level set value and velocity, respectively.

to the unbalanced net force induced by the wettability difference, leading to asymmetric spreading, and an air cavity is formed in the center. In the retracting stage, the liquid on the left of the hydrophobic area rapidly recoils toward the impact center, forming the tilt shape shown at 6.6 ms. In addition, the high-speed jet ejection reported in the literature [54] is observed here. At 8.0 ms, rapid retraction of the left part of the liquid leads to detaching and directional migration toward the hydrophilic area.

From Fig. 5, the droplet exhibits partial bouncing behavior only for the case with a small wettability difference $\Delta\theta_e = 30^\circ$; on the other hand, for cases with a greater wettability difference, droplets move directionally without leaving the surface. The velocity field comparison in Fig. 8 demonstrates that retracting flow leaves the surface almost perpendicularly for the case $\Delta\theta_e = 30^\circ$, whereas complex inner flow such as swirling flow, shown as the red curve, is observed at 11.8 and 15 ms for the case $\Delta\theta_e = 60^\circ$. It is caused by the larger velocity difference in the retracting flows on different wetting surfaces. The retracting flow from the hydrophobic region moves toward the more wettable area with a higher lateral velocity, inducing the liquid cap to move to the right rather than leave the surface vertically. Thus, the increase in the wettability difference decreases the droplet height and lowers the probability of the droplet bouncing from the surface.

The changes in the maximum and minimum positions of the TPCL measured from the sectional view are plotted in Fig. 9. Here we define the “spreading diameter” as the difference between the maximum and minimum positions of the TPCL, because the contacting area is not circular in these cases. Following the initial asymmetric spreading stage (before 2.5 ms), the contact line in the nonwetting area retracts rapidly toward the borderline (from 2.5 ms to approximately 11.0 ms), while it is pinned on the surface after a slight movement in the wetting region. At this point, the

FIG. 8. Sectional views of the velocity field comparing the droplet rebounding and sticking behavior on the surface with wettability difference at 30° and 60° . Images and arrows are colored by the level set value and velocity value same as that in Fig. 7, respectively.

FIG. 9. The contact line position (x axis) of the impinging droplet on the left hydrophobic (L) and the right hydrophilic (R) areas. The black dashed line represents the borderline in Fig. 1.

FIG. 10. The duration of droplet contact with the left hydrophobic region at different wettability difference. Images show the droplet appearance when it just leaves the nonwetting surface.

droplet detaches itself from the left hydrophobic region and directionally migrates to the hydrophilic area. For the case $\Delta\theta_e = 120^\circ$, the extreme wettability difference leads to the farthest position of the TPCL on the wettable surface. It is emphasized here that the net force in the lateral direction imposed by the unbalanced lateral forces from both sides induces this directional rebounding and migration of the water droplet toward the hydrophilic area [27].

The contact time, defined as the duration of droplet contact with the left hydrophobic region, is shown in Fig. 10 at different wettability differences. It can be found that increasing the wettability difference reduces the contact time between the liquid and the nonwetting area, which is due to the increase in the unbalanced net force in the lateral direction in accordance with the equation $dF_Y = \sigma(\cos\theta_A - \cos\theta_B)dx$. Theoretically, during the droplet-wall interaction process, two stages (spreading and retracting) can be observed. According to Eq. (16) for spreading [55] and Eq. (17) for retracting [56], both values (t_s and t_r) decrease with the increase of contact angle θ_{app} : spreading time [55]

$$t_s = \frac{2}{3} \sqrt{\frac{D_0}{\rho_l \mu u_0}} \left(\frac{\rho_l D_0^3 u_0^2 + 12 D_0^2 \sigma}{D_{\max} u_0^2} - \frac{2 D_{\max} [1 - \cos(\theta_{app})] \sigma}{u_0^2} \right), \quad (16)$$

retracting time ($We \gg 1$) [56]

$$t_r \propto \frac{D_{\max}}{U_{\text{ret}}} \approx 2 \sqrt{\frac{\rho_l D_0^3}{8 \sigma}} (\sqrt{\pi [1 - \cos(\theta_{app})]})^{-1}, \quad (17)$$

where U_{ret} is the retraction velocity of the contact line, $D_{\max}$ is the maximum spreading diameter of the droplet, which has been well studied in various articles and one of theoretical formulations

FIG. 11. Time evolution of impinging water droplets with varying We from 1 to 30, corresponding to u_0 from 0.19 m/s to 1.04 m/s, on the substrate with $\Delta\theta_e = 60^\circ$ and offset = 0.0.

related to the contact angle was expressed as [57]

$$\frac{D_{\max}}{D_0} = \sqrt{\frac{We + 12}{3[1 - \cos(\theta_{\text{app}})] + 4We/\sqrt{Re}}}, \quad (18)$$

where Re is the Reynolds number. When we combine Eq. (16) with Eq. (18), an increasing contact angle leads to a decrease of t_s . In addition, the t_r also decrease with the rise of contact angle according to Eq. (17). Therefore, when the wettability difference increases from 30° to 120° in Fig. 10, the contact time ($t_s + t_r$) between the droplet and the hydrophobic part goes down.

B. Weber number effect

In Fig. 11, the influence of We values from 1 to 30 on droplet deformation and directional migration is shown. It is observed that as We increases, the spreading diameter at 3.2 ms increases and the migration distance of the droplet at 20 ms increases. As We increases, the impinging droplet has much more kinetic energy to rapidly spread and retract after touching the surface. In addition, the migration distance of the droplets increases as We increases. At extremely high We values, droplet split by the borderline is predicted. It occurs because of the significant difference of the spreading and recoiling behavior between the hydrophobic and the hydrophilic regions. Subsequently, the liquid in the hydrophobic area moves rapidly toward the wetting region and reunites with the liquid sticking in the hydrophilic area at approximately 10.0 ms.

To provide deeper insight into the We effect, Fig. 12 shows the evolution of the contact line position on the surface. During the asymmetric spreading stage, the spreading diameter increases as We increases. However, no significant difference is observed during the retracting, detaching, and migrating stages for We values of 1, 10, and 20. For cases with a We value of 30, an extremely different detaching behavior is observed due to the droplet splitting behavior. Referring to the images in Fig. 11, the bridge (at 6.0 ms) connecting the two parts of the liquid recoils to the left hydrophobic area (at 8.0 ms), leading to a quick change in the contact line position. At 10 ms, the rapid recoiling bridge induces rebounding of the liquid in the hydrophobic area, which is shown in Fig. 12 as a rapid change in the contact line position.

FIG. 12. The contact line position (x axis) of the impinging droplet on the left hydrophobic (L) and the right hydrophilic (R) areas. The black dashed line represents the borderline in Fig. 1.

The effect of We on the contact time is plotted in Fig. 13. For cases with We values from 1 to 20, the contact time first increases and then decreases, whereas the contact time for $We = 30$ is relatively large. On a specific uniform surface, indeed, the contact time is not dependent of the impact velocity u_0 but a function of D_0 , ρ_l , and σ [49]. However, there is another key parameter in this work—the wettability difference ($\Delta\theta_e$), which exerts a significant effect on the contact time because of the different spreading and retracting behaviors of liquid on two kinds of surfaces. On surfaces with a wettability difference, the unbalanced Young’s force always drives the liquid towards the more wetting area, leading to the asymmetric spreading behavior of droplets. Moreover, the contact line on the left hydrophobic area moves largely to the left upon the increase of We from 1 to 10 ($0.2 \leq u_0 \leq 0.6$ m/s) shown in Fig. 12 owing to the dynamic wetting [58], whereas only a small increase is seen from $We = 10$ –30 ($0.6 \leq u_0 \leq 1.04$ m/s) [59]. Subsequently, the recoiling behaviors of liquid on two surfaces make a further difference. An experimental result [60] demonstrated that capillary mode dominates the retraction process for both hydrophobic and hydrophilic surfaces under small We ($We \leq 10$), whereas the inertial rate increase rapidly for droplet recoiling on hydrophobic surfaces with We from 10 to 100.

Hence, according to the spreading and retracting behaviors of droplets on different wetting surfaces, the curve in Fig. 13 shows increased behavior for We smaller than 10 due to the rapid spreading, and then it decreases owing to the combined effect of inertial and capillary retraction of liquid on hydrophobic surface. As for the very long contact time under $We = 30$, it occurs because the droplet is split by the borderline (see Fig. 11) that the unbalanced Young’s force cannot continue to drag the liquid on hydrophobic surfaces towards more wetting area. Thus, the contact time between droplet and the left hydrophobic surface is larger than that under small We conditions.

FIG. 13. The duration of droplet contact with the left hydrophobic region at different We . Images show the droplet appearance when it just leaves the nonwetting surface.

C. Effect of offset impinging

The behavior of a water droplet on a substrate with offset impinging is illustrated in Fig. 14. With negative offset impingement, the great part of the droplet in the hydrophobic area directionally rebounds, whereas the other part of the liquid still remains on the surface at 9.6 ms, and the droplet almost leaves the surface at 13.2 ms. With positive offset impinging, a small part of the liquid spreads in and rapidly detaches from the hydrophobic area at 6.0 ms. Finally, the droplet pins in the hydrophilic area. In the experiment conducted in Ref. [27], various droplet behaviors with positive offset impinging such as directional rebounding and the landing distance were investigated experimentally on substrates with moderate and extreme wettability differences. Simulation results with

FIG. 14. Time evolution of impinging water droplets with different offsets, and fixed wettability difference at 60° and $We = 10$.

FIG. 15. Top view exhibiting the comparisons of the droplet surface profiles (upper half) and the velocity fields (lower half) at the early retracting stage with different offsets. The liquid surface and the velocity fields are colored by velocity in x axis.

three different offset impinging schemes in the present study facilitate a complete understanding of the effect of the wettability difference on droplet behaviors.

In Fig. 15, the top view images at 4.0 ms compare the droplet shape and velocity field for different offset impinging schemes. The upper-half profile indicates that offset impinging has a significant effect on the droplet shape, which results in limited spreading of liquid in the hydrophobic area. The red- and blue-colored regions on the droplet surface indicate the high- and low-velocity positions, respectively. The velocity direction illustrates that the liquid on both sides retracts to the impact center, but the rapid recoiling liquid in the nonwetting area induces droplet directional migration. An interesting question is whether the thin liquid film in the impact center ruptures or not. A perfect liquid film can be captured by the current grid scheme in the wetting region, but film rupture occurs in the hydrophobic area due to the nonwetting surface property. This is not discussed in the present paper because no significant effect of the film on droplet spreading and retracting was observed, as described by the validation section in our previous work [36].

V. CONCLUSION

The effects of the surface wettability difference, Weber number (We), and offset impinging on droplet asymmetric spreading and direction migration were studied computationally using a DNS/CLSVOF interface-tracking method. The mesh-dependent contact angle was employed for the boundary condition. The numerical method was validated comprehensively for a simple droplet impacting and spreading on a homogeneous surface with varying ECAs. Extensive simulations were performed to examine the droplet motion and the deformation on heterogeneous surfaces.

It was observed that the droplet underwent asymmetric spreading, retracting, detaching, and migrating phases when it impacted on a surface with a wettability difference, which was different from the four stages a droplet passed through after impinging on homogeneous surfaces. The asymmetric spreading behavior of the droplet was caused by the unbalanced net force in the lateral direction. Directional rebounding toward the more wetting area was induced by the rapid retraction of the liquid in the hydrophobic area. The increase in the wettability difference led to farther transport of the contact line, decrease in the droplet bouncing height, and a shorter contact time between the liquid and the non-wetting area.

It was also found that the droplet spreading diameter was significantly affected by We , because a larger kinetic energy caused the liquid to spread further. For the duration of the droplet contact with the hydrophobic area, however, no large difference was observed during the retracting and detaching stage for We values of 1, 10, and 20, which was attributed to the combined effect of the spreading diameter and the surface tension. The distance between the contact line position and the borderline increased as We increased. When the droplet impacted with a high We value of 30, droplet splitting was observed, leading to a larger contact time than that without the splitting

behavior. Finally, simulation results revealed that offset impinging plays a major role in droplet spreading and deformation.

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