Droplet impact simulation with Cahn–Hilliard phase field method coupling Navier-slip boundary and dynamic contact angle model

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Physics of Fluids 36, 042115 (2024)
https://doi.org/10.1063/5.0202604
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ABSTRACT
As a highly promising interface capture tool, the phase field method (PFM) has gained fast development in the past 20 years or so including in the simulation of droplet impact. The mobility tuning parameter $\chi$ of PFM, however, is hard to determine since it ambiguously reflects the relative strength between advection and diffuse effects that are difficult to quantify. This problem becomes even more complex when it is coupled with the contact line movement modeling, i.e., the dynamic contact angle (DCA) model, which is closely related to the effective slip ($L_{se}$) and the Navier-slip ($L_s$). This study systematically investigated the factors that would take effect at the interface capture and the contact line movement in droplet impact simulation. The value and the scaling law of $L_{se}$ as for its dependence on $\chi$ and interface thickness ($\varepsilon$) was first confirmed, and an approximation scheme for defining the DCA model was proposed based on the difference between the apparent contact line moving velocity ($U_{cl}$) and the Navier-slip velocity at the contact line ($U_{0cl}$), which is inherently determined by $L_{se}$ and $L_s$, respectively. After validation with the experiments, the scaling law of $\chi$ with $\varepsilon$, i.e., the sharp-interface limit, was finally obtained, which provides improved droplet impact simulation.

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I. INTRODUCTION
Droplet impact dynamics simulation normally involves two aspects, i.e., how to capture the water–air interface, i.e., the interface, and how to model the motion of the contact line, i.e., the triple line among water, air, and the solid boundary. In terms of the interface capture methods, two different approaches have been successfully established, i.e., the sharp-interface model as represented by the volume of fluid (VOF) method and the diffuse-interface model as represented by the phase field method (PFM). The sharp-interface model assumes the interface to be with zero thickness, while the diffuse-interface model assumes the interface with a finite thickness. The VOF method has the inherent drawback in describing the surface tension and sometimes needs to incorporate extra models such as the continuum surface force (CSF) model. This brings higher requirements for the capture of interface curvature, especially when the curvature of the interface is on the same scale as the interface thickness. This troublesome problem could be eliminated in PFM as it employs the gradient of the free energy inside the interface to calculate surface tension. Therefore, PFM owns the advantage in surface tension modeling, especially when the interface deforms abruptly in a small region.

The fundamental theories about PFM could be traced back to the work of Van der Waals who first proposed the concept of diffuse interface, then Cahn–Hilliard developed the well-known Cahn–Hilliard equation (CH equation) to describe the deformation and motion of the interface driven by the free energy variation in the interface. Since around 2000, advances in mathematics and computing method have accelerated the application of PFM in multiphase flow simulations. For instance, Gurtin et al. and Ren and Weinan systematically analyzed the thermodynamic continuity problem of the CH equation coupled with the Navier-stokes equation (CH-NS equation), Badalassi et al. proposed a semi-implicit discrete scheme to solve the CH-NS equation, Lowengrub and Truskinovsky suggested a smoothing scheme for the phase field diffusion interface, Yue et al. successively developed the concise expression of surface tension in PFM from different perspectives based on the Cahn–Hilliard free energy theory. Consequently, PFM has been successfully applied in a plenty of multiphase flow simulations, including...
However, PFM is not a perfect scheme, which relies on the tuning of two key parameters: the interface thickness, i.e., \( \varepsilon \) (m), which determines the resolution and the precision of the simulation, and the mobility parameter, \( \gamma = \rho c^2 \) (m/s/kg), or equivalently the mobility tuning parameter \( \chi \) (m/s/kg), which determines the timescale of the interface thermodynamic equilibrium. For \( \varepsilon \), the main concern is to achieve a satisfactory precision without costing too much computing resources, it is normally reflected by the Cahn number, i.e., \( C_h = \varepsilon / L_c \), representing the relative scale between the artificially set \( \varepsilon \) and the characteristic length of the system, i.e., \( L_c \). It has been well proved that \( C_h \approx 0.01 \) is a proper choice. While in terms of \( \chi \), it is more complex and must be chosen judiciously. Because \( \chi \) resembles the local mass transport at the interface between two phases, it determines the timescale of the interface thermodynamic relaxation. It must be sufficiently large to retain a constant interfacial thickness but small enough so that the convective terms are not overly damped. When it is taken too small and the system is more controlled by advection, this could thin or thicken the interface and thus destroy the thermodynamic equilibrium at the interface. This can be avoided by using a higher mobility parameter, because the surface tension cannot be established precisely and steadily unless the interface reaches a thermodynamic equilibrium state. To the best of the authors’ understanding, the role of mobility could be qualitatively interpreted as it determines the strength of “numerical surface tension,” which tries to keep the thermodynamic equilibrium of the diffuse interface when advection effect, such as the inertia flow, tries to break it. Conversely, the mobility parameter cannot be too large otherwise it will damp the advection flow. Normally, the Pélet number is used

\[
P_c = \frac{U_c \varepsilon}{\gamma \sigma} = \frac{U_c \varepsilon}{\mu \sigma} = \frac{U_c \varepsilon}{\rho \chi L_c}.
\]

with \( U_c \) being the characteristic velocity of the system and acted as the reference for the proper choice of \( \chi \) because \( Pe \) resembles the relative strength of advection over diffuse of the system. The proper choice of \( \chi \) is then related to an important concept in PFM, i.e., the sharp-interface limit, which means that with a proper scaling law of \( C_h \) or \( Pe \), the simulation results would be independent of \( \varepsilon \). Therefore, it could not be simply interpreted as only about \( \varepsilon \) being as small as possible to reach a sharp-interface limit, it is more about the proper choice of \( \chi \) when \( \varepsilon \) varies in a reasonable range. Unfortunately, the scale law of \( C_h \) or \( Pe \) or \( \chi \) being has yet not reached an agreement in both theoretical analysis and simulation practices. For instance, Lowengrub and Truskinovskiy first proposed \( Pe \propto 1/C_h \) or \( Pe \propto 1/C_h^2 \) based on the quasi-incompressible model. Jacqmin then concluded based on diffusion, interface tensor, and chemical potential analysis that \( \gamma \propto \varepsilon^2 \) with \( 1 \leq \varepsilon < 2 \), i.e., when \( \varepsilon = 1 \), \( Pe \) is constant, and when \( \varepsilon = 2 \), \( Pe \propto 1/C_h^{\frac{1}{2}} \). Verschueren assumed when \( \varepsilon \) approaches zero, \( Pe \propto C_h^{\frac{3}{2}} \). Khatavkar et al. took the characteristic length scale in the definition of \( Pe \) as \( \varepsilon \), i.e., if \( Pe = U_c \varepsilon^2 / \gamma \sigma \), then \( Pe \propto C_h^{\frac{1}{2}} \). The more recent research by Maggetti also suggested that when \( \varepsilon \) approaches zero, \( Pe \propto 1/C_h^{\frac{3}{2}} \). Corresponding to the above theoretical analysis, Bai et al.’s recent work on the occurrence of microdroplets showed that within the range of 0.025 < \( C_h < 0.04 \), \( Pe \propto C_h^{\frac{1}{2}} \). Zanella et al.’s research on Rayleigh instability has yielded different conclusions that as \( C_h \) approaches 0.02, \( Pe \propto 1/C_h^{\frac{1}{2}} \). However, in terms of the \( C_h \) or \( Pe \) or \( \chi \) scaling law in droplet impact problems, to the best of the authors’ knowledge, the related discussion or experimentation is very limited. Also, the investigations so far in terms of the scaling law have been confined to the physical system with the same relative strength of advection-diffuse effects, when the system properties change, for instance, when the droplet impacts with different diameter or velocity, the related discussions is still empty.

The discussion above is mainly about the air–water interface capture, while in droplet impact simulation, the modeling about the contact line movement is even more complex. First of all, whether the boundary should be considered as no-slip or partial slip has gained a long-history debate. The classical no-slip boundary assumes the velocity on the boundary is always zero, but would fail in contact line problems because it would induce the stress singularity at the contact line. To avoid it, slip boundary was introduced and developed as represented by the Navier-slip boundary, which allows a finite velocity along the boundary calculated by

\[
U_{\text{bound}} = L_c \frac{dU}{dy},
\]

where \( U_{\text{bound}} \) is the velocity on the boundary, \( L_c \) is the slip length, and \( dU/dy \) is the velocity gradient near the boundary in the vertical direction.

However, when the dynamic contact angle (DCA) model is applied in PFM, Navier-slip becomes sometimes necessary. In droplet impact, the contact angle varies during its spreading and receding processes under the competition among inertia effect, surface tension, and solid surface wetting property, which is far different from the static contact angle given by the Young’s equation. Generally, the DCA model could be developed by experimentally measured advancing contact angle \( \theta_a \), the static contact angle \( \theta_s \), and the receding contact angle \( \theta_r \). DCA model has been demonstrated necessary and effective by a plenty of simulation works and there are several DCA models wildly applied, such as Kistler model, Blake model, and Yokoi et al. model. Even though they differ in format or mathematical mechanism, most of them take the dynamic contact angle \( \theta_d \) as a function of the contact line moving velocity \( U_{\text{cl}} \). Conventional VOF models tend to use no-slip boundary and replace \( U_{\text{cl}} \) by an “equivalent velocity,” such as by the velocity in the neighborhood mesh cells. Similar approach in PFM has yet not been reported.
but it is assumed to be even more challenging because different from sharp-interface type methods, the diffuse interface in PFM crosses several mesh grids which would then bring more trouble for deciding where to take the equivalent velocity.

To better simulate droplet impact, it becomes desirable to couple PFM/Navier-slip/DCA model, but several issues need to be clarified beforehand, including the value and scaling law of $L_s, \epsilon$ how to properly define the DCA model on the basis of the relationship between $L_s, \epsilon$ and $u_0$, and the scaling law of $\chi$. With these questions in mind, this study aims to draw a whole picture by applying a coupled PFM/Navier-slip/DCA model in droplet impact simulations, with the intention to decouple the interactions among the three modules. The Navier-slip boundary was proposed to directly capture $U_{cl}$ on the exact boundary, which would be beneficial in avoiding bringing in more numerical models to capture the “neighborhood velocity,” the underlying difference between $U_{cl}$ and $U_d$ that originated from the difference between $L_s, \epsilon$ and $L_a$ are clarified.

II. METHODOLOGY

A. Phase field method and Navier-slip boundary

In the PFM diffuse interface with a finite thickness $\epsilon$, a dimensionless phase field variable $\phi$ is defined and goes from 0 to 1 in the interface, and the volume fraction of individual fluid is defined as

$$V_{f1} = \frac{1 - \phi}{2}, \quad V_{f2} = \frac{1 + \phi}{2},$$

respectively, the density $\rho$ and the viscosity $\mu$ of the mixture vary smoothly across the interface as

$$\rho = \rho_1 + (\rho_2 - \rho_1)V_{f2}, \quad \mu = \mu_1 + (\mu_2 - \mu_1)V_{f2}. \quad (2)$$

The Cahn–Hilliard equation is split into

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{u} \nabla \phi = \nabla \cdot \left( \gamma \frac{$$\phi^2 - 1}{$$\phi^2 + 1} \phi \right),$$

where $\mathbf{u}$ is the fluid velocity field and $\lambda$ is the mixing energy density. The following equation relates the mixing energy density and the interface thickness to the surface tension: \(\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \nabla \cdot \left( \gamma \phi \right). \quad (3)

The transport and conservation of mass and momentum in PFM are governed by the Navier–Stokes equation as

$$\rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{F_d} + \rho g,$$ \quad (5)

where $\mathbf{F_d}$ is the diffuse interface surface tension, governed by the variation of free energy in the interface as

$$\mathbf{F_d} = G \nabla \nabla \phi,$$ \quad (6)

and $G$ is chemical potential such that

$$G = \delta \left[ -\nabla \phi^2 + \phi \frac{(\phi^2 - 1)}{\epsilon^2} \right],$$ \quad (7)

with $\delta$ being the Dirac $\delta$ function that is only non-zero at the interface.

For the boundary condition, it is defined as

$$\mathbf{n}_{bound} \cdot \mathbf{n}_{bound} = 0,$$

and the value of the velocity on the boundary is given by the Navier-slip boundary as

$$U_{bound} = L_a \frac{dU}{dy}.$$ \quad (9)

The viscous boundary friction could be expressed by

$$F_v = -\mu \frac{dU}{dy} = -U_{bound} \frac{dU}{L_s dy}.$$ \quad (10)

The DCA model is applied by

$$F_d = \delta \left( \mathbf{n}_{bound} \mathbf{n} - \cos \theta_d \mathbf{n} \right),$$ \quad (11)

where $\mathbf{n}_{bound}$ is the normal vector of the boundary, $\mathbf{n}$ is the normal vector of the interface near the boundary, and $\delta$ is the Dirac function that is only non-zero at the contact line on the boundary. Therefore, $F_d$ indicates a force to correct the direction of the interface near the contact line to meet the predefined contact angle.

B. Dynamic contact model

The DCA model adopted in this study was the classical Kistler model, where $\theta_d$ is defined by

$$\theta_d = f_{Hoff} \left[ 0.0138 U_{cl} + f_{Hoff}^2 \theta_{eq} \right], \quad (12)$$

with $f_{Hoff}$ being the Hoffman function \( (9) \) given by

$$f_{Hoff} = \frac{\cos \left[ \frac{1}{1 + \frac{1.13x}{0.76}} \right]}{1 + \frac{1.13x}{0.76}}.$$ \quad (13)

In the spreading process $\theta_{eq} = \theta_{a_{max}}$ and in the receding process $\theta_{eq} = \theta_{r_{max}}$, where $\theta_{a_{max}}$ is the minimum advancing contact angle and $\theta_{r_{max}}$ is the maximum receding contact angle, both should be measured when the contact line remains still. Figure 1 shows the Kistler model with $[\theta_{a_{min}}, \theta_a, \theta_{r_{max}}] = [90°, 55°, 37°]$ as measured in the present work where the droplet impacts on a medium-hydrophilic silicon wafer surface, and the error of contact angle measurement was ±2°. Theoretically, $\theta_d$ transfers from $\theta_{a_{min}}$ to $\theta_{r_{max}}$ with $U_d = 0$, i.e., the contact line remains motionless during the transition, which would physically link to the concept of contact angle hysteresis. Also one could notice the Yokoi model differently allows the transition from $\theta_{a_{min}}$ to $\theta_{r_{max}}$ with a finite $U_d$ instead of $U_d = 0$. Therefore, considering this would be sometimes difficult to precisely measure $U_d$ when it is close to 0, as similarly depicted in Ref. 80, to the best of the pixel-resolution of the high-speed camera captured pictures, the $[\theta_{a_{min}}, \theta_{r_{max}}] = [90°, 37°]$ was actually identified with $U_d = 0.01$–0.02 m/s. However, considering the trend of the function as shown in Fig. 1 where $\theta_d$ varies quite slowly around $U_d = 0$, so the error of the identification of $\theta_{a_{min}}$ and $\theta_{r_{max}}$ could be neglected. Here, the critical $U_d$ when $\theta_d = \theta_{a_{max}}$ and $\theta_d = \theta_{r_{max}}$ was defined as $U_a$ and $U_r$, respectively, and it is reasonable to assume $U_a \leq 0.01$ m/s and $U_r \geq 0.01$ m/s.

However, it needs to be carefully clarified that in the definition of DCA models, the contact line velocity $U_{cl}$ means the macroscopic
contact line moving velocity, when applying the Navier-slip boundary and capturing the contact line velocity on the exact boundary, i.e., $U_{cl}$, then the difference between $U_{cl}$ and $U_{0cl}$ should be carefully considered before defining the DCA model with $U_{0cl}$ in simulation.

Consider the tiny zone near the contact line, $U'_{cl}$ is determined by the velocity gradient $dU/dy$ by

$$U'_{cl} = L_s \frac{dU}{dy}. \quad (14)$$

Here the $dU/dy$ should not be considered as usual like the result calculated by flow field in one phase, but would be determined by the interface diffuse effect, i.e., the effective slip:

$$dU = U_{cl} \frac{dU}{L_{s,e}}. \quad (15)$$

Therefore,

$$U'_{cl} = U_{cl} \frac{L_s}{L_{s,e}}. \quad (16)$$

As could be seen, the DCA model in simulation could not be directly defined as experiment results but would be regulated by the ratio between $L_s$ and $L_{s,e}$, which is defined as $R_s$. For easier understanding, in the following text, $U_{cl}$ represents the apparent contact line moving velocity, and $U'_{cl}$ represents the Navier-slip velocity along the boundary at the location of the contact line.

**C. Experiment and simulation model description**

The initial droplet radius was $D_0 = 2.5$ mm, the impact velocity was $V_0 = 1.5$ m/s, and the experiments of droplet impact dynamics
were recorded by a high-speed camera (i-speed 703, ix-cameras) with the frame rate of 25 000 f/s, at the pixel resolution of 800 × 640. From experiment, as shown in Fig. 2(a), the inertia-driving fast spreading reaches its maximum, i.e., \( \beta_{\text{in}} = 3.16 \pm 0.06 \) at \( t_{\text{in}} = 3.6 \pm 0.2 \text{ ms} \) where the spreading factor \( \beta \) was defined as \( \frac{D(t)}{D_0} \) and then stayed in the transition zone where \( \theta_\text{a} \) transferred from \( \theta_{\text{a, min}} \) to \( \theta_{\text{a, max}} \) with the contact line almost motionless, and the time duration was \( t_{\text{f}} = 1.0 \pm 0.1 \text{ ms} \). During 4.6–19.4 ms, the contact line receded with almost a uniform velocity, i.e., \( \overline{U_{\text{cl}, r}} = 0.126 \text{ m/s} \), and after \( t = 19.4 \text{ ms} \), the contact line settled at \( \beta_{\text{f}} = 1.67 \pm 0.05 \). Figure 2(b) shows the sketch of the simulation model, equilateral-triangle mesh was applied over the whole domain including the area near the boundary for easier comparison between cases, and the characteristic size of the mesh was denoted as \( h_c \).

### III. RESULTS AND DISCUSSION

#### A. The scaling law of \( L_{s,e} \) with \( c_{\chi} \) and \( \varepsilon \)

Before carrying out the simulations, the value of \( L_{s,e} \) and its relationship with \( \chi \) and \( \varepsilon \) should be identified in order to properly define and apply the DCA model later. As mentioned earlier, the estimation of \( L_{s,e} \) remains some disputes. To find out the exact value of \( L_{s,e} \), a pretest with no slip boundary and a static contact angle of 45° was implemented.

![Graph showing the relationship between \( L_{s,e} \) and \( \chi \) with \( \alpha \) varying from \( 1 \) to \( 10 \text{ m/s/kg} \).](image1)

![Graph showing the relationship between \( U_{\text{cl}, r} \) and \( \chi \).](image2)

![Graph showing the relationship between \( dU/dy \) and \( \chi \).](image3)

![Graph showing the relationship between \( L_{s,e} \) and \( \varepsilon \).](image4)
FIG. 5. Simulation results with the DCA model by experiment measurement. (a) The comparison of \( \beta \) between experiment and simulation. (b) The dynamic contact angle along the process extracted from simulation. \( C_h = 0.01, L_s = 1500\) nm, \( \chi = 8\) m/s/kg.

FIG. 6. Simulation results with the DCA model by 10 times shrinkage of the horizontal ordinate of experiment measurement. (a) The DCA model. (b) The zoom-in view of the contact angle transition zone, i.e., the zone enclosed by the red dashed line in (a). (c) The comparison of \( \beta \) between experiment and simulation. (b) The dynamic contact angle along the process extracted from simulation. \( C_h = 0.01, L_s = 1500\) nm, \( \chi = 8\) m/s/kg.
Here, the fixed contact angle of 45° was meaningless since the target was to find $L_{s,e}$ by $L_{s,e} = U_{cl}/(dU/dy)$. As shown in Fig. 3, where the results of the spreading factor $\beta$, the contact line moving velocity $U_{cl}$, and the velocity gradient at the contact line on the boundary $dU/dy$ were extracted. For all in Fig. 3, $D_0 = 2.5 \text{ mm}$, $V_0 = 1.5 \text{ m/s}$, $\varepsilon = 0.01 \text{ D}_0 = 25 \mu \text{ m}$, i.e., $C_h = 0.01$, and $\chi$ investigated ranged from 1 to 10 m/s/kg, the data were taken during $t = 10.0\text{−}15.0 \text{ ms}$ where the receding velocity $U_{cl,r}$ was almost uniform. The results show obvious irrelevance between $L_{s,e}$ and $\varepsilon$ and the average value of $L_{s,e}$ for $\varepsilon = 25 \mu \text{ m}$ is $\varepsilon = 14.8 \mu \text{ m}$. We further extended the investigation of the relationship between $L_{s,e}$ and $\varepsilon$ with $\varepsilon = 1\text{−}10 \text{ m/s/kg}$ and the average value of $L_{s,e}$ varying with $C_h (\varepsilon)$ is shown in Fig. 4. Apparently, $L_{s,e}$ shows strong linear relationship with $C_h (\varepsilon)$, and the linear fitting coefficient was identified as 0.59, i.e.,

$$L_{s,e} = 0.59 \varepsilon.$$  \hspace{1cm} (17)

To summarize, the results agree with Ding’s conclusion that $L_{s,e}$ is independent from $\chi$ but would be proportional to $\varepsilon$, and the coefficient found in the present study is different from Ding, which might be resulted from the different range of $\varepsilon$ investigated.

B. The approximation scheme for defining DCA

Combining Eqs. (16) and (17), one could obtain

$$U_{cl} = U_{cl} = \frac{L_{s,e}}{0.59 \varepsilon}.$$  \hspace{1cm} (18)

For instance, if $L_s$ is taken as 1500 nm and $\varepsilon = 25 \mu \text{ m}$, i.e., $C_h = 0.01$, corresponding to $R_s = 0.1$, there would exist one order-of-magnitude difference between $U_{cl}$ and $U_{cl}$. Thus the DCA model found from the experiment and fitted by Kistler model, i.e., the model shown in Fig. 1 is not applicable anymore. As a proof, Fig. 5 shows the results where the DCA model in Fig. 1 was used, i.e., $[\theta_{\alpha,\text{min}}, \theta_{\alpha}, \theta_{\text{r, max}}] = [90°, 55°, 37°]$ and $[U_{\alpha}, U_r] = [0.01, -0.01]$ m/s, by taking $C_h = 0.01$, $L_s = 1500 \text{ nm}$, $\chi = 8 \text{ m/s/kg}$ as an example.

As shown in Fig. 5(a), the simulation results could not well match the experiment and the reason would be the incorrect application of DCA model. Figure 5(b) shows the dynamic contact angle extracted from simulation and that the contact angle transition process was much longer than experiment, i.e., $t_t = 2.2 \text{ ms}$ compared with $t_t = 1.0 \text{ ms}$ in the experiment, and the contact angle in receding is...
around 36° which is also inconsistent with the experiment that for \( U_{dl'} = 0.126 \text{ m/s}, \theta_{dl'} = 30° \) according to Fig. 1. The difference between \( U_{dl'} \) and \( U_{di} \), i.e., \( U_{dl'} \) is around ten times smaller than \( U_{di} \) should be responsible for the two divergences mentioned above.

Then one may assume to zoom in the whole horizontal ordinate by a factor of \( R_s \) in Fig. 1 to compensate for the difference between \( U_{dl'} \) and \( U_{di} \), while this would induce numerical sensitiveness problems. For instance, as shown in Fig. 6 where the DCA model was defined on \( U_{dl'} = 0.1 U_{di} \), i.e., the whole horizontal ordinate in Fig. 1 was shrunk by 10 times [Figs. 6(a) and 6(b)], the simulation results could not satisfy the experiment either [Fig. 6(c)]. The reason is the variation trend of \( \theta_{dl} \) with \( U_{dl'} \) becomes overly intense especially in the receding process, considering the droplet receding process is not ideal with a uniform velocity, the contact angle fluctuates intensely, as shown in Fig. 6(d).

Therefore, considering the droplet spreads with almost a constant value of \( \theta_{dl} = \theta_{dl_{min}} = 90° \), except for the first 1 ms or so whose influence could be neglected, and recedes with an average value of \( \theta_{dl} = \theta_{dl_{max}} = 30° \), here an approximation scheme was proposed to define the DCA model by replacing \([\theta_{dl_{min}}, \theta_{dl_{max}}]\) with \([\theta_{dl}, \theta_{dl}]\) to model the main process of spreading and receding respectively, and by replacing \([U_{dl}, U_{di}]\) with \([U_{dl}' = U_{dl} R_s, U_{di}' = U_{di} R_s]\) to model the contact angle transition zone. The corresponding DCA model can be seen in Figs. 7(a) and 7(b). Taking \( \theta_{dl} = 0.1, U_{dl}' = 0.001 \text{ m/s}, U_{di}' = -0.001 \text{ m/s} \), \([\theta_{dl}, \theta_{dl}] = [90°, 30°]\), it turned out when \( \chi \) was taken as 8 m s/kg, the simulation results agreed well with experiment results, as shown in Figs. 7(c) and 8 (Multimedia available online), and Fig. 7(d) exhibits the dynamic contact angle varying with time extracted from simulation results, which agrees well with the DCA model in Fig. 1 and the experiment observation that the transition zone lasts for \( t_i \approx 0.9 \text{ ms} \) and the contact angle in spreading is around 90° and in receding is between 28 and 31°.

To further validate the effectiveness and robustness of the proposed approximation scheme for defining the DCA model, cases with \( L_s \) in the same-scale as 1500 nm, i.e., \( L_s = 1000 \) and 2000 nm and trans-scale, i.e., \( L_s = 10 \) and 100 nm were calculated. Here, \( U_{dl}' = -U_{di}' = 0.001 \text{ m/s} \) for \( L_s = 1000 \) and 2000 nm, \( U_{dl}' = U_{di}' = 1 \times 10^{-4} \text{ m/s} \) for \( L_s = 100 \text{ nm} \), \( U_{dl}' = -U_{di}' = 1 \times 10^{-5} \text{ m/s} \) for \( L_s = 10 \text{ nm} \) to maintain \( U_{dl}' = U_{dl} R_s, U_{di}' = U_{di} R_s \), the results could be found in Fig. 9(a). Apparently, the scheme shows fine robustness. The optimal value of \( \chi \), i.e., \( \chi_{opt} \) for \( L_s = 1000, 1500, \) and 2000 nm is 9, 8, and 8 m s/kg respectively, and the difference could be neglected.

Also, the possible experimental measurement error of \( U_{dl}/U_{di} \) or \( U_{dl}'/U_{di}' \) was proved no worry that when \( L_s = 1500 \text{ nm} \) and other conditions were kept the same, for \( U_{dl}' = -U_{di}' = 1 \times 10^{-2}, 1 \times 10^{-4}, \) and \( 1 \times 10^{-5} \text{ m/s} \), the simulation results were all quite satisfactory, as

\[
\begin{align*}
\text{FIG. 8.} & \quad \text{Comparison between simulation and experiment with typical snapshots and video.} \\
\text{FIG. 9.} & \quad \text{Proof of the robustness of the proposed approximation scheme for defining DCA.}
\end{align*}
\]

\[
\begin{align*}
\text{FIG. 8.} & \quad \text{Comparison between simulation and experiment with typical snapshots and video.} \\
\text{FIG. 9.} & \quad \text{Proof of the robustness of the proposed approximation scheme for defining DCA.}
\end{align*}
\]
FIG. 11. Effect of Ls by viscous friction force near the boundary when a droplet impacts on a superhydrophobic surface. (a) and (b) The SEM image and the 3D height map of the micro-channel structure of the superhydrophobic surface respectively. (c) The static contact angle measurement result. (d)--(g) Ls needs to be large enough to avoid the internal flow near the spreading out-rim being overly restrained by the viscous boundary friction thus inducing an undesirable outcome. The tilting of the out-rim would happen when $L_s/h_c = 1$ (d) while would not when $L_s/h_c = 10$ (e). (f) and (g) The internal flow field of (d) and (e) at t = 0.8 ms, respectively. For (d)--(g), air is denoted in blue and water in red. The white arrows in (f) and (g) represent the internal flow and its length if proportional to the value of velocity.

FIG. 10. Exhibition of the liquid film rapture when Ls is taken too large for the medium hydrophilic surface. Air is denoted in blue and water in red.
shown in Fig. 9(b). In the following text, the approximation scheme was adopted.

C. The effect of Lₙ to the internal flow by viscous effect

Although it has been clear so far that the role of Lₙ is mainly in properly defining DCA model, it does not mean Lₙ would never dramatically influence the simulation results by the viscous friction force, i.e., $F_r$. Figure 10 exhibits the results of $Lₙ = 1.67L_{α,e}$ = 25 μm, with $C_h = 0.01$ and $χ = 8$ m s/kg, $U'_l = -U'_l = 0.01$ m/s. As could be seen, the overly unconstrained internal flow would lead to a much thinner liquid film before and after the maximum spreading was reached, which would then easily crush unless the interface thickness be further refined. For $C_h = 0.005$–0.01, according to our study, $L/h_c$ = 0.5 is the upper limit.

The influence of $Lₙ$ to internal flow through its regulation of viscous friction near the boundary is even more significant when the droplet impacts on a superhydrophobic surface, that $Lₙ$ needs to be large enough to avoid the internal flow being overly restrained near the boundary. Figures 11(a) and 11(b) exhibit the SEM image and the three-dimensional (3D) height map of the micro-channel structured surface fabricated with laser ablation method, the contact angle of the superhydrophobic surface is $[θ_a, θ_s, θ_r] = [165°, 161°, 158°]$ and the measurement result of the static contact angle is shown in Fig. 11(c). When $Lₙ = 25$ μm, i.e., $L/h_c = 1$, the spreading out-rim would get lifted off the surface during spreading at $t = 0.9$ ms, i.e., the tilting phenomenon of the spreading out-rim, as shown in Fig. 11(d), while this distortion could be eliminated by a larger $Lₙ$ as shown in Fig. 11(e) where $Lₙ = 250$ μm, i.e., $L/h_c = 10$. Figures 11(g) and 11(h) present the flow field near the spreading out-rim at $t = 0.8$ ms for $Lₙ = 25$ μm and $Lₙ = 250$ μm respectively, where the change of internal flow direction could be clearly observed between them. The comparison between simulation and experiment for a droplet impacting on the superhydrophobic surface with $D_0 = 2.5$ mm, $V_0 = 1.5$ m/s, $[θ_a, θ_s] = [165°, 161°, 158°]$, $C_h = 0.01$, $Lₙ = 250$ μm, $χ = 9$ m s/kg is shown in Fig. 12 (Multimedia available online).

Therefore, to conclude, the principle of choosing the proper value of Navier-slip length, i.e., $Lₙ$ includes:

1. For medium hydrophilic/hydrophobic surfaces, $Lₙ$ should be properly chosen to correctly impose the DCA model together with $L_{α,e}$, but should not be too large to avoid the internal flow being overly unconstrained. $L/h_c < 0.1$ is recommended.
2. For superhydrophobic surface, $Lₙ$ should be large enough to avoid the internal flow near the boundary being overly damped thus inducing the failure of correctly calculating the spreading dynamics, $L/h_c$ on the scale of 10 is recommended.

Interestingly, the difference in the order of proper $Lₙ$ for medium-hydrophilic surface and superhydrophobic surface found here is

![Experiment](image)

**FIG. 12.** The comparison between simulation and experiment on superhydrophobic surface. $D_0 = 2.5$ mm, $V_0 = 1.5$ m/s, $C_h = 0.01$, $Lₙ = 250$ μm, $χ = 9$ m s/kg. In the third row, air is denoted in blue and water in red. Multimedia available online.
FIG. 13. The effect of $v$ on simulation results. (a) Results of $\beta$ vary with time when $v$ is between 1 and 10 m s $^{-1}$/kg. (b) The dynamic contact angle extracted from the simulation which is independent of $v$ and all agree well with the experiment results. (c) and (d) The effect of $v$ to $r_t/r$, (c) $v = 1$ m s $^{-1}$/kg, (d) $v = 10$ m s $^{-1}$/kg, and the time line is same for both. For all, $C_h = 0.01$, $L_s = 1000$ nm, $U_0 = \frac{-U_f}{1 \times 10^{-3}}$ m/s.
somehow in accordance with experimental or MD simulation results that the real slip length on superhydrophobic surfaces would be hundreds or even thousands of times larger than that on hydrophilic surfaces.82–84

D. The effect of $\chi$ to simulation results and the scaling law of $\chi$-$\varepsilon$

After the value and scaling law of $\chi$-$\varepsilon$ being clarified and subsequently the approximation scheme of DCA model being proved accurate, we further investigated the effect of $\chi$ where the theoretical descriptions and its scaling law with $\varepsilon$ are somehow unclear.

Figure 13(a) exhibits the results affected by $\chi$ with $C_h = 0.01$, $L_s = 1000$ nm, $U_0 = 1 \times 10^{-3}$ m/s. The dynamic contact angle is independent with $\chi$ as shown in Fig. 13(b), which consists of the results shown in Fig. 3. Obviously, the influence is mainly presented during the receding process since the spreading is more dominated by the inertia effect, and the receding velocity $U_{cl,r}$ would increase with $\chi$.

By assuming the receding is mainly driven by the diffuse interface $F_{st}$ as described in Eqs. (6) and (7), while is not directly correlated with $\chi$, it would be more intuitive to show the effect of $\chi$ to $\nabla \phi$. As shown in Figs. 13(c) and 13(d),

FIG. 14. Scaling law of $\chi$-$\varepsilon$ for a given system. For all, $D_0 = 2.5$ mm, $V_0 = 1.5$ m/s, and the simulation setting was kept the same by keeping $\varepsilon = \frac{h_c}{R_s}$, $R_s$ = constant, $U_0 = -U_r = 1 \times 10^{-3}$ m/s.

FIG. 15. Scaling law of $\chi$-$\varepsilon$ between different systems with the comparison of $\beta$-$\varepsilon$ between simulation and experiment results. For all, the simulation model setting was kept exactly the same with the case of $[D_0, V_0] = [2.5$ mm, $1.5$ m/s] as shown in Figs. 7 and 8, including the $\varepsilon$, $h_c$, $L_s$, and the DCA model.
FIG. 16. Comparison between simulation and experiment results with snapshots and video for the scaling law of $\chi - \epsilon$ between different systems. For all, the simulation model setting was kept exactly the same with the case of $[D_0, V_0] = [2.5 \text{ mm}, 1.5 \text{ m/s}]$ as shown in Figs. 7 and 8, including the $\nu$, $h_L$, $L_s$, and the DCA model. (a)–(d) $[D_0, V_0] = [2.5, 2.25]$, $[2.5, 0.72]$, $[3.26, 1.5]$, and $[2.02, 1.5]$ (mm, m/s), respectively, and in the third row of them, air is denoted in blue and water in red. Multimedia available online.
\[ \nabla \phi = \sqrt{ (\partial \phi / \partial \eta)^2 + (\partial \phi / \partial \zeta)^2 } , \]  
(19)

and the results of \( \nabla \phi \) when \( \chi = 1 \text{ m s/kg} \) and \( \chi = 10 \text{ m s/kg} \) in several typical moments are compared. As indicated, \( \nabla \phi \) is more stable during the whole process for \( \chi = 10 \text{ m s/kg} \) while showing certain variation when \( \chi = 1 \text{ m s/kg} \), and between the receding process, \( \nabla \phi \) for \( \chi = 1 \text{ m s/kg} \) is around 25% smaller than it is for \( \chi = 10 \text{ m s/kg} \). The reason could be explained by the relative strength between advection and diffusion. When \( \chi \) is taken too small, and the advection effect is more dominant, the interface could not keep a stable thickness from being disturbed by advection, then the local interface would be widened thus \( \nabla \phi \) would decrease, which in turn leads to the reduction of \( F_{se} \). This explanation could be further demonstrated by the area enclosed within the red line frame in the second row in Fig. 13(c), for instance, that at \( t = 1.0 \text{ ms} \) when the inertia/advection effect is high, the interface thickness is severely enlarged to form a blurred area.

Next, the scaling law of \( \chi - \varepsilon \) in the range of \( C_h \leq 0.01 \) was identified from two aspects. First of all, with the same droplet impact condition, i.e., the same \( D_0 \) and \( V_0 \), and similar model setting, i.e., by keeping \( \varepsilon = h_c \), \( h_c = \) constant, and applying the same DCA model. It turns out that \( \chi = 8 \text{ m s/kg} \), for \( C_h = 0.0025, 0.005, 0.0075, \) and 0.01, the simulation results are all quite satisfactory, and the results could be seen in Fig. 14. This implies that when \( C_h \) approaches 0 for a given system, \( \chi \) should be kept as constant, that is, \( Pe \propto 1/C_h \), which supports the argument of Lowengrub and Truskinovsky,12 Jacqmin,26 and Magaletti et al.25

However, when the relative strength between advection and diffusion of the system varies physically, i.e., when the droplet impacts with different \( D_0 \) and \( V_0 \), the scaling law above is not applicable anymore. To prove it, four more groups of experiments and simulations were conducted, i.e., \([D_0, V_0] = [2.5, 2.25], [2.5, 0.72], [3.26, 1.5], \) and \([2.02, 1.5] \) (mm, m/s), respectively, it turns out that \( \chi_{opt} \) increases with \( D_0 \times V_0 \) instead of being a constant. Specifically, \( \chi_{opt} = 12.4, 11.6 \) (m s/kg), respectively, i.e., \( \chi_{opt} \propto D_0 \times V_0 \). And the comparisons between simulation and experiment results could be seen in Figs. 15 and 16 (Multimedia available online). For the simulations of them, the model setting is strictly the same as the case of \([D_0, V_0] = [2.5 \text{ mm}, 1.5 \text{ m/s}] \) as discussed above, to eliminate any possible errors brought by the mesh, the internal flow, the boundary velocity calculation and the DCA model. The reason that \( \chi_{opt} \) is proportional to \( D_0 \times V_0 \) instead of being a constant is because for a larger droplet or a higher impact velocity, physically the advection effect strengthens. Hence, for a given \( \varepsilon \), PFM needs a higher mobility \( \chi \) to resist the stronger distortion effect on the interface from advection to keep its thermodynamic equilibrium and stable thickness.

Therefore, by combining the validation from two aspects, it could be finally obtained that:

1. For a given system \((D_0 \times V_0 = \text{constant})\), when \( C_h \) approaches 0 in the range of \( 0.0025-0.01 \), \( \chi_{opt} = \text{constant} \), i.e., \( Pe \propto 1/C_h \).
2. Between different systems \((D_0 \times V_0 \text{ varies})\), \( \chi_{opt} \propto D_0 \times V_0 \), i.e., \( Pe \) should be kept as a constant.

IV. CONCLUSION

On the basis of rigorous validation with experiments, the general principles in utilizing PFM/Navier-slip/DCA model in droplet simulations were clarified in this work. The main novelty and contribution may include:

(1) Two theoretically disputed scaling laws, i.e., the scaling law of the effective slip length \( L_{se} \) with mobility tuning parameter \( \chi \) and interface thickness \( \varepsilon \), and the scaling law of \( \chi \) with \( \varepsilon \) were validated and appropriately extended.

(2) An approximation scheme for defining the dynamic contact angle was proposed, by adopting the characteristic dynamic contact angle during the spreading and receding phases as \( \theta_{sl, s} \) and \( \theta_{sl, r} \), respectively, and the transition process was scaled by the relationship between the apparent contact line moving velocity \( U_d \) and Navier-slip velocity \( U_{sl} \), which inherently correlated with the Effective slip length \( L_{se} \) and artificially set Navier-slip length \( L_s \).

(3) The effect of Navier-slip on the internal flow by viscous effect near the boundary and the proper value range were identified for both medium hydrophilic and superhydrophobic surface.

The findings in this work advance our understanding of the phase field method, the Navier-slip boundary, and the dynamic contact angle model and provide guidance for parameter choice in droplet impact simulations. The systemic simulation scheme proposed in this study would be worthwhile to try for problems involving droplets, impacting onto a solid surface. It shall be cautious that the findings of this study might not be universally applicable, but only valid in the range of \( 0.0025 \leq C_h \leq 0.01 \). Further theoretical work would be highly encouraged.

ACKNOWLEDGMENTS

This work was supported by NSFC-DFG Mobility Programme (No. M-0368).

AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Zuru Fu: Conceptualization (lead); Data curation (lead); Formal analysis (lead); Methodology (lead); Writing – original draft (lead).

Haichuan Jin: Software (equal); Guice Yao: Data curation (equal); Software (equal); Validation (equal). Dongsheng Wen: Funding acquisition (lead); Resources (lead); Supervision (lead); Writing – review & editing (lead).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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