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Key points

- The mesoscopic phase-field model reproduces both the hydrodynamic and the molecular kinetic models for wetting dynamics on solid substrates.
- A computational strategy is provided for computing realistic flows.
- Contact angle hysteresis can be easily incorporated into the phase-field model.

Abstract

The wetting dynamics on solid surfaces has been a long-standing problem, since the traditional sharp-interface Navier-Stokes formulation encounters a non-integrable stress singularity at the contact line. In recent years, the phase-field model, which regularizes the contact-line singularity by Cahn-Hilliard diffusion, has gained increasing popularity in wetting simulations, and this article offers an up-to-date review of this approach. In this model, the contact line is moved by diffusion and the contact angle condition is enforced by a wall energy. The governing equations satisfy a dissipative energy law, which guarantees the fulfillment of the second law of thermodynamics. If properly implemented, this model is consistent with the Cox theory in terms of the apparent contact angle and with the molecular kinetic theory in terms of the dynamic contact angle. By exploiting the competition between the Cahn-Hilliard diffusion and the wall energy relaxation, we provide a computational strategy for simulating realistic flows at affordable computational cost. A simple modification of the wall energy relaxation equation extends the model to contact angle hysteresis. Some applications of the phase-field model are provided in the end.

Introduction

The three-phase contact line is perhaps the most significant unresolved problem in multiphase flows. In static equilibrium, the static or equilibrium contact angle θ_S subtended by the interface and the solid surface satisfies the well-known Young's equation $\sigma \cos \theta_S = \sigma_{w2} - \sigma_{w1}$, where σ , σ_{w1} , and σ_{w2} are interfacial tensions between the two fluids and the solid substrate, as shown in Fig. 1A. When fluid 1 steadily displaces fluid 2 with a velocity *V*, the problem runs into a singularity at the contact line, where the contact line moves with *V* but the fluid velocity is supposed to vanish due to the classical non-slip boundary condition. It is generally agreed that the difficulty arises from the fact that microscopic physics dominates the local behavior at the contact line, and the continuum Navier-Stokes formulation fails to represent that. Hydrodynamic and molecular kinetic theories have been developed to describe the local dynamics at the contact line, with the aim to predict the experimentally measurable apparent contact angle θ_M (see Fig. 1B) as a function of the contact line velocity *V*.¹

The hydrodynamic theory, exemplified by the Voinov-Cox matched asymptotic solution,^{2,3} introduces a slip length to carve out the immediate neighborhood of the contact line from the hydrodynamic domain. Thus a fluid-mechanical solution can be obtained in the outer region while the stress singularity can be relieved by the slip model in the inner region. The key results from this type of

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Fig. 1 Schematics of (A) a static contact line and (B) a dynamic contact line. θ_D is the (microscopic) dynamic contact angle, which may be different from the static contact angle θ_S . θ_M is a suitably defined (macroscopic) apparent contact angle.

analysis are the following. First, the outer solution is insensitive to the slip models.⁴ The upside of this recognition is that a faithful description of the local dynamics is unnecessary for an accurate solution of the macroscopic flow. The downside is that measurements, limited to larger length scales, would be ineffective in elucidating the local dynamics. Second, the apparent contact angle θ_M is determined by viscous bending in such a manner³:

$$g(\theta_M) = g(\theta_S) + Ca \ln(\delta^{-1}), \tag{1}$$

where *g* is function given by Cox^3 and $\delta = l_s/W$ is the ratio between the slip length l_s and the macroscopic length *W*. The capillary number $Ca = \mu V/\sigma$, where μ is a characteristic fluid viscosity, indicates the strength of viscous bending relative to the surface tension σ . In this model, the microscopic contact angle remains θ_s , i.e., $\theta_D = \theta_s$ in Fig. 1, and bending of the interface mainly occurs in an intermediate region between the inner region of scale l_s and the outer region of scale *W*. This formula has been corroborated by experimental observations of drop spreading on a highly wettable surface,^{5,6} but fails to represent data of liquid-liquid displacement.⁷

The molecular kinetic theory (MKT),⁸ on the other hand, treats the motion of the contact line as the consequence of molecules jumping from one interface to another. Different from the hydrodynamic theory where the dissipation is caused by viscosity, the dissipation in MKT occurs at the molecular level. As a result, the MKT predicts the microscopic dynamic contact angle θ_D instead of the macroscopic angle θ_M .

The possibility of reconciling and perhaps integrating the two approaches have been discussed by Blake.¹ The phase-field model, also known as the diffuse-interface model, is an alternative attempt at integrating the micro- and macroscopic scales. This model was first proposed for critical-point wetting by Cahn⁹ in 1979 and its Cahn-Hilliard version has been especially popular in the simulation of contact line problems, e.g., Refs. 10–16. In this work, we will focus on the Cahn-Hilliard model and use the terms phase-field and Cahn-Hilliard interchangeably. The phase-field model treats the interface as a diffuse and continuous layer. By expanding the density distribution function and then truncating the nonlocal intermolecular forces, one coarse-grains the microscopic physics at the contact line into fluid-fluid and fluid-substrate interfacial energies, which are then incorporated into the continuum hydrodynamic model. On this mesoscopic scale, the motion of the contact line is effected by diffusion across the interface and there is no singularity. In fact, the phase-field model integrates both the hydrodynamic and the molecular kinetic models. On the one hand, the Cahn-Hilliard model has a diffusion length *l*_D that is connected to slip length *l*_s in slip models.¹⁷ Consequently, the predicted θ_M can accurately match the Cox theory **Eq. (1)**. On the other hand, the wall energy relaxation yields a θ_D that agrees with the MKT, at least in the leading order.¹⁸

In reality, most solid surfaces are intrinsically rough or chemically heterogeneous. As a consequence, the contact line may get pinned at the topological or chemical defects and results in non-unique values in the static contact angle, which is known as the contact angle hysteresis (CAH). The maximum and minimum static contact angles are referred to as the advancing (θ_A) and receding (θ_R) angles.^{19,20} Of course, contact angle hysteresis can be computationally reproduced if topological or chemical heterogeneities on the solid wall are sufficiently resolved, ^{16,21,22} but this can be very costly, especially when the heterogeneity scale is much smaller than the macroscopic scale. It is computationally more favorable to treat the rough surface as smooth with θ_A and θ_R as input parameters. The wall energy relaxation can be easily extended to accommodate θ_A and θ_R , which makes the phase-field model a promising tool for computing contact line problems with CAH.

In this review, we will focus on our previous work and provide our own understanding on the phase-field model for the moving contact line problem. We will first give the complete formulation. Then we will discuss the sharp-interface limit and the computational strategy for realistic flows. After that we will discuss the simple modification to the wall energy relaxation equation, which enables the phase-field model for CAH. Finally, we will provide some numerical examples involving viscoelastic fluids, rough surfaces, and CAH.

Phase-field formulation

For an incompressible two-phase system of Newtonian fluids in contact with a solid wall, we introduce a phase-field variable ϕ , which changes smoothly from +1 in fluid 1 to -1 in fluid 2. The fluid interface is diffuse and stores a mixing energy²³

$$f_m(\phi, \nabla \phi) = \lambda \left(\frac{1}{2} |\nabla \phi|^2 + f_0(\phi) \right), \tag{2}$$

where λ is the mixing energy density, $f_0(\phi) = \frac{(\phi^2 - 1)^2}{4\epsilon^2}$ is a double-well potential, and ϵ is a capillary width characterizing the interfacial thickness. A one-dimensional interface at equilibrium assumes a hyperbolic tangent profile $\phi(x) = \tanh\left(\frac{x}{\sqrt{2e}}\right)$, and the region of $\phi \in [-0.9, 0.9]$ has a thickness of 4.164 ϵ . The equivalence of the mixing energy for the diffuse interface and the surface tension σ for the corresponding sharp interface gives $\sigma = \frac{2\sqrt{2}}{3} \frac{\lambda}{\epsilon}^{24}$. The wetting property of the solid surface can be described by the wall energy

$$f_w(\phi) = -\sigma \cos \theta_S \frac{\phi(3-\phi^2)}{4} + \frac{\sigma_{w1} + \sigma_{w2}}{2},$$
(3)

which reproduces the fluid-solid interfacial tensions σ_{w1} and σ_{w2} (see Fig. 1A) for $\phi = 1$ and -1, respectively. It should be noted that the value of $\frac{\sigma_{w1}+\sigma_{w2}}{2}$ does not matter since the governing equations only contain $f'_w(\phi)$. The minimization of the free energy $\int_{\Omega} f_m d\mathbf{x} + \int_{\partial \Omega_w} f_w ds$, where Ω denotes the computational domain and $\partial \Omega_w$ denotes the solid wall boundary, reproduces Young's equation $\sigma \cos \theta_S = \sigma_{w2} - \sigma_{w1}$.

The governing equations for the two-phase flow can be written as

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) + \mathbf{J} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \mathbf{G} \nabla \phi + \rho \mathbf{g},\tag{4}$$

$$\nabla \cdot \mathbf{u} = \mathbf{0},\tag{5}$$

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \nabla \cdot (M \nabla G), \tag{6}$$

$$G = \lambda \left(-\Delta \phi + f_0'(\phi) \right), \tag{7}$$

where ρ is the density, **u** is the volume-averaged velocity, $\tau = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ is the viscous stress, μ is the viscosity, *G* is the chemical potential, **g** is the gravitational acceleration, and *M* is the mobility parameter. The Cahn-Hilliard equation is split into two second-order Eqs. (6) and (7), which is a common treatment in finite element methods^{14,25} because the *C*⁰ finite elements cannot handle fourth order derivatives directly. It should be noted that the additional term $\mathbf{J} = \frac{\rho_2 - \rho_1}{2} M \nabla G$ is a diffusive flux caused by the discrepancy between **u** and the mass-averaged velocity.^{26,27} This term takes action only in the diffuse interface and has negligible effect if the diffuse interface is thin enough. Thus this term has been ignored in many simulations that focus on the physical problem.

These equations are complemented by the following boundary conditions on the solid surface:

$$\mathbf{u} = \mathbf{u}_w,\tag{8}$$

$$\mathbf{n} \cdot \nabla G = \mathbf{0},\tag{9}$$

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = -\Gamma L(\phi, \nabla \phi), \tag{10}$$

where \mathbf{u}_w is the wall velocity, Γ is a positive phenomenological parameter that controls the rate of wall energy relaxation, and

$$L(\phi, \nabla \phi) = \lambda \mathbf{n} \cdot \nabla \phi + f'_{w}(\phi) \tag{11}$$

is the wall potential. Eqs. (8–10) correspond to the no-slip, zero diffusive flux, and wall energy relaxation conditions, respectively. It should be noted that the dynamic contact angle θ_D may deviate from θ_S , and $\theta_D = \theta_S$ is recovered only when Eq. (10) is replaced with $L(\phi, \nabla \phi) = 0$.¹⁷

The governing Eqs. (4–7) with conditions Eqs. (8–10) on the solid surface and proper conditions on other boundaries (such that these boundaries do not do any work to the system) satisfy the following dissipative energy law:

$$\frac{d}{dt}\mathscr{F} = -\int_{\Omega} (M|\nabla G|^2 + \tau : \nabla \mathbf{u}) d\Omega - \int_{\partial \Omega_w} \Gamma L^2 ds,$$
(12)

where $\mathscr{F} = \int_{\Omega} \left(f_m(\phi, \nabla \phi) + \frac{1}{2}\rho |\mathbf{u}|^2 \right) d\mathbf{x} + \int_{\partial \Omega_w} f_w(\phi) ds$ is the total free energy of the system, Ω denotes the computational domain and $\partial \Omega_w$ denotes the solid surface. Physically, this dissipative energy law guarantees the system is consistent with the second law of thermal dynamics. Numerically, it can be used to guide the construction of energy-stable numerical schemes.^{28,29}

Phase-field parameters for contact line dynamics

For a two-phase system, the interfacial tension σ and static contact angle θ_S can be experimentally measured. But the phase-field model has some additional parameters to be determined: ε , M, and Γ . In order to capture the correct contact line dynamics, it is crucial to understand the roles played by these parameters, which correspond to the following three dimensionless groups:

$$Cn = \frac{\varepsilon}{W} (\text{Cahn number}),$$
$$S = \frac{\sqrt{M\mu}}{W},$$
$$\Pi = \frac{1}{W},$$

 $\overline{\mu \Gamma W}$

where *W* is the characteristic macroscopic length scale. Note that the model parameter λ can be obtained from σ and ε .

Ideally, we should choose ε based on the physical thickness of the fluid-fluid interface, which is of molecular scale. In order to numerically resolve the diffuse interface, we have to distribute $1 \sim 2$ cells over ε across the diffuse interface,^{24,25} which means ε cannot be arbitrarily small. A typical numerical simulation can only resolve the Cahn number down to $Cn \sim 0.001$ even with local mesh refinement at the interface. Thus it is more practical to choose ε based on the computational power, and then choose *M* and Γ in a way such that the numerical result is no longer sensitive to ε and approaches a sharp-interface limit with sufficient accuracy.

It is evident from Eq. (6) that the mobility parameter *M* controls the interfacial diffusion, which plays a key role in moving the contact line. Based on a scaling argument, Yue et al.¹⁷ identified a so-called diffusion length $l_D = \sqrt{M\mu}$, which characterizes the inner contact line region in the phase-field context. This length scale was also noted earlier by Jacqmin¹¹ based on dimensions. Fig. 2A plots the velocity field near the contact line in a Poiseuille flow, with one fluid displacing another in a planar channel under a pressure gradient. The reference frame is affixed to the steady-state interface such that the wall moves to the left. The contact line region features a stagnation point of distance $D \approx 2.5 l_D$ from the wall, which plays a similar role as the slip length l_s in slip models. This equivalence is further evidenced by the comparison with the matched asymptotic analysis by Cox as shown in Fig. 2B. Despite using different devices to regularize the contact-line singularity, the phase-field model generates essentially the same macroscopic flow as the slip model with $l_s = 2.5 l_D$. Experimentally, one can extract l_s by fitting the Cox theory to experimental data such as drop spreading measurements.³⁰ Then we can use the phase-field model to reproduce the contact line dynamics using l_D (or *M*) predicted by l_s . For systems with a large viscosity contrast, numerical experiments show that the geometric average of the two viscosities should be used to compute l_D .¹⁷

A key concept in using the phase-field models is to achieve the so-called sharp-interface limit.^{31,32} Matching the realistic values of the interfacial thickness can be prohibitively expensive, thus creating a numerical difficulty. Through systematic numerical experiments, Yue et al.¹⁷ suggests the following criterion for the contact line dynamics to approach the sharp-interface limit with sufficient accuracy: $\varepsilon < 4l_D$ or Cn < 4S. This criterion guarantees that the flow field at the contact line, as shown in Fig. 2A, can be adequately resolved. However, the physically meaningful diffusion length, typically at the order of nanometers to microns, is much smaller than the macroscopic length, typically at the order of millimeters or greater. This poses a technical difficulty to be resolved later using wall energy relaxation.

We now turn to the wall relaxation parameter Γ . It is well-known that the wall energy relaxation Eq. (10) allows the microscopic dynamic contact angle θ_D to deviate from the static one θ_S . For a planar interface that insects the solid wall at angle θ_D , the wall potential Eq. (11) can be rewritten as²⁷

$$L(\phi, \nabla \phi) = \frac{3}{4} \sigma \left(1 - \phi^2 \right) (\cos \theta_D - \cos \theta_S), \tag{13}$$

where we have assumed the equilibrium hyperbolic tangent profile of ϕ such that $|\nabla \phi| = \frac{1-\phi^2}{\sqrt{2\varepsilon}}$. If the steady contact line motion is very slow such that the diffuse interface maintains its equilibrium profile, then Eq. (10) leads to a quantitative relation between θ_D and the contact line velocity *V*:

$$\frac{\cos\theta_{\rm S} - \cos\theta_{\rm D}}{\sin\theta_{\rm D}} = \frac{V}{\Gamma\lambda} = \frac{2\sqrt{2}}{3} \frac{V}{\Gamma\varepsilon\sigma}.$$
(14)

For $\theta_D \approx 90^\circ$, this relation reduces to the linear form of Blake's MKT¹:

$$\cos\theta_S - \cos\theta_D = \frac{\zeta V}{\sigma},\tag{15}$$

where $\zeta = \frac{2\sqrt{2}}{3} \frac{1}{\Gamma_e}$ is the so-called contact line friction, which has been adopted by Amberg and coworkers.^{33,34}

According to the Cox theory, the viscous force outside the inner contact-line region bends the interface such that the interface angle varies from θ_S at the wall to the apparent contact angle at the macroscopic length scale *W*. Increasing l_s (or equivalent l_D) effectively reduces the shear rate and thus reduces the bending of the interface. However, the wall energy relaxation, which rotates the interface at the contact line from θ_S to θ_D , can exactly compensate the reduction in viscous bending. This has been confirmed by





Fig. 2 Phase-field simulation of contact line dynamics in Poiseuille flow. (A) The typical velocity field near the contact line as captured by the phase-field model. The frame is fixed to the contact line that moves steadily. The solid lines are the level sets of $\phi = \pm 0.9$, and the black dot indicates the stagnation point. $Ca = \frac{\mu V}{\sigma} = 0.02$, where μ is the viscosity of the advancing fluid. (B) Comparison of apparent contact angle with the Cox theory.³ $\delta = \frac{l_s}{W}$, where l_s is the slip length characterizing the inner region of the contact line. No wall energy relaxation is considered, i.e., $\Pi = \frac{1}{\mu \Gamma W} = 0$. (C) Fitting experimental data by adjusting wall energy relaxation. The symbols are from experiments on glycerin displacing silicone oil in a capillary by Fermigier and Jenffer.⁷ The following common parameters are used unless otherwise specified in the plots: $\theta_S = 98^\circ$, receding-to-advancing viscosity ratio of 0.9, $Cn = \frac{e}{W} = 0.01$, and $S = \frac{l_w}{W} = 0.01$. Here *W* is the half-width of the channel. (A) and (B) reprinted with permission from Ref. 17. Copyright 2010, Cambridge University Press. (C) Adapted with permission from Ref. 18. Copyright 2011, American Institute of Physics.

numerical experiments in Ref. 18: the drop spreading curves for different l_D collapse into a master curve as long as Γ is properly chosen. Under restricted conditions, such as $\theta_D \approx 90^\circ$ and equal viscosities, we only need to choose Γ according to

$$\frac{1}{\mu\Gamma\varepsilon} = 5.97 \ln\left(\frac{l_D}{\tilde{l}_D}\right) \tag{16}$$

in order to reproduce the contact line dynamics with a physical diffusion length $\tilde{l}_D \ll l_D$. For the general case, the relation above is no longer valid and Γ has to be used as a tuning parameter to fit the experimental data.

Now we provide a computational strategy for choosing the phase-field parameters in order to capture the moving contact lines in experiments. First, we pick an affordable ε . On the one hand, the lower bound of ε is limited by the minimum mesh size. On the other, ε has to be small enough, ideally $Cn \leq 0.01$, such that the interfacial dynamics is insensitive to variations of ε . Second, we

determine *M* such that $l_D \ge \varepsilon/4$ to achieve the sharp-interface limit of contact line dynamics. This l_D is usually much greater than the physical \tilde{l}_D that corresponds to the slip length suggested by experiments. Finally, we fit one experimental data point to determine Γ or equivalently the dimensionless group Π . The parameters *M* and Γ thus determined will be able to reproduce all other experimental data points and even predict contact line dynamics in other geometries. In the whole simulation, Γ is the only fitting parameter, with a similar role as l_s in slip models. A similar strategy that uses Γ , in the form of the contact line friction, as the fitting parameter has also been adopted by Carlson et al.^{33,35,36}

Fig. 2C shows an implementation of this computational strategy. We first pick an affordable ε with Cn = 0.01. Then we choose $l_D = \varepsilon$ (i.e., S = Cn) such that $l_D > \varepsilon/4$. Then we tune Γ to match the critical *Ca* where wetting failure occurs in the experiment, which gives $\Pi = 0.67$ as the optimal fitting parameter. By fixing S = 0.01 and $\Pi = 0.67$, the phase-field method is able to reproduce experimental data for a wide range of *Ca*. It should be noted that this computational strategy is insensitive to the choice of *S*: for a different choice of $S = 3.16 \times 10^{-3}$, the experimental data can still be equally reproduced, but with a different Π . More discussions on the sharp-interface limit and the computational strategy for contact line computations can be found in Refs. 17,18,37.

It should be noted that the slip condition can also be included in the phase-field model as a generalized Navier boundary condition (GNBC).^{13,38} In the GNBC, a slip velocity that is proportional to the sum of the viscous shear stress and the unbalanced Young's stress is introduced. With properly chosen parameters, the velocity profile near the vicinity of the contact line can match that from molecular dynamics simulations. This condition, however, introduces an additional slip coefficient, which brings extra difficulty to parameter determination. Besides, the difference between the GNBC and the no-slip condition is only limited to the contact line region, and there is no evidence showing that one condition outperforms the other in terms of contact line dynamics at the macroscopic level.

Contact angle hysteresis

When CAH exists, the static contact angle has non-unique values, the maximum of which is the advancing contact angle θ_A and the minimum of which is the receding contact angle θ_R . The contact line advances if $\theta_D > \theta_A$, recedes if $\theta_D < \theta_R$, and is pinned if $\theta_R \le \theta_D \le \theta_A$, as illustrated in Fig. 3.

Since θ_D is already embedded in the wall potential as shown in Eq. (13), the wall energy relaxation equation of Eq. (10) can be easily modified to include contact angle hysteresis. For example, we may include the contact angle θ as a parameter in the definition of f_w and L^{27} :

$$L(\phi, \nabla \phi; \theta) = \lambda \mathbf{n} \cdot \nabla \phi - \frac{3}{4} \sigma \cos \theta (1 - \phi^2), \qquad (17)$$

where θ can be either θ_A or θ_R . It is obvious that $L(\phi, \nabla \phi; \theta_A) > L(\phi, \nabla \phi; \theta_R)$ since $\phi \in [-1, 1]$ and $\theta_A > \theta_R$. If the diffuse interface does not deviate much from its equilibrium profile, then Eq. (17) can be approximated by

$$L(\phi, \nabla \phi; \theta) = \frac{3}{4} \sigma \left(1 - \phi^2 \right) (\cos \theta_D - \cos \theta)$$
(18)

following Eq. (13). We can easily see that $L(\phi, \nabla \phi; \theta) > 0 \Leftrightarrow \theta_D < \theta$ and $L(\phi, \nabla \phi; \theta) < 0 \Leftrightarrow \theta_D > \theta$. Thus the state of the contact line can be connected to the signs of $L_A = L(\phi, \nabla \phi; \theta_A)$ and $L_R = L(\phi, \nabla \phi; \theta_R)$:

- advancing contact line: $\theta_D > \theta_A \Leftrightarrow 0 > L_A > L_R$;
- receding contact line: $\theta_D < \theta_R \Leftrightarrow L_A > L_R > 0$;
- pinned contact line: $\theta_A \ge \theta_D \ge \theta_R \Leftrightarrow L_A \ge 0 \ge L_R$.

Further considering that the advancing contact line dynamics is controlled by L_A and the receding contact line by L_R , we come to the extended wall energy relaxation equation

$$\frac{\partial \phi}{\partial t} + \cdot \nabla \phi = -\Gamma \text{minmod} (L_A, L_R), \tag{19}$$



Fig. 3 Three states of a contact line with CAH. Reprinted with permission from Ref. 27. Copyright 2020, Cambridge University Press.

where minmod(a, b) = $\begin{cases} sign(a)min(|a|, |b|) & \text{if } ab > 0 \\ 0 & \text{otherwise} \end{cases}$. This equation switches automatically between the three states without

the explicit knowledge of θ_D . More importantly, the governing equations with Eq. (10) being replaced by Eq. (19) maintains an energy law similar to Eq. (12), but with an additional dissipation term due to CAH. For a contact line that advances and then recedes (or recedes and then advances) back to its original position, this additional dissipation is exactly $\sigma(\cos \theta_R - \cos \theta_A)A$, where *A* is the surface area swept by the contact line. More discussions on CAH can be found in Ref. 27.

In Ref. 34, Amberg employed a contact line friction $\frac{1}{\Gamma_{\ell}}$ that is dependent on θ_D . By imposing a very large contact line friction for $\theta_D \in [\theta_R, \theta_A]$ to slow down the contact line motion, one can capture the major features of contact angle hysteresis. But this approach requires the evaluation of θ_D and, more importantly, the contact line cannot be exactly pinned.

Applications

The phase-field method has been widely used in a variety of wetting problems: wicking and droplet imbibition in microchannels,^{39,40} breakup of liquid drops and filaments on partially wetting solid substrates,^{41,42} coalescence induced droplet jumping,^{43–47} and water entry problem,⁴⁸ just to name a few from our own work. Here we will pick three problems where the fluid rheology or surface properties play important roles on the wetting dynamics.

Wetting dynamics of viscoelastic fluids

In many industrial applications, such as coating, inkjet printing, and enhanced oil recovery, the fluids are non-Newtonian. Fluid rheology is known to affect the interfacial dynamics away from the contact line. The strong straining flow in the inner region of the contact line can further highlight the non-Newtonian effect. For example, Garoff and co-workers observed experimentally that the non-Newtonian effect was confined to the close vicinity of the contact line when a cylinder was pushed into a bath of polymer liquid.^{49,50} In this inner region, the viscous bending of interface is reduced by shear thinning and enhanced by viscoelasticity. There are also experiments indicating that contact line motion is enhanced by both shear thinning and viscoelasticity.⁵¹ The effect of shear thinning is easy to understand, while that of viscoelasticity cannot be rationalized intuitively. We will therefore focus on viscoelasticity in the following.

In order to study the effect of viscoelasticity, it is essential to capture the strong straining flow at contact line. The phase-field model offers a unique advantage in this regard, as evidenced by the strong shear flow between the stagnation point and the solid wall (see Fig. 2A), which is otherwise absent in slip models that have been widely adopted in other popular numerical methods such as volume-of-fluid,^{52,53} level-set,^{54,55} and immersed boundary⁵⁶ methods. Fig. 4 shows the typical distribution of polymer



Fig. 4 Contours of the *xx* component of the dimensionless polymer stress $\tau_{pxx}/\left(\mu \frac{V}{W}\right)$ when a viscoelastic fluid displaces a Newtonian fluid in a 2D channel. The two thick lines, being the level sets of $\phi = \pm 0.9$, roughly mark the boundaries of the diffuse interface. The advancing fluid (to the left of the interface) is viscoelastic, and the receding fluid (to the right of the interface) is Newtonian. $\theta_S = 90^\circ$, $S = \frac{I_0}{W} = 0.01$, $Ca = \frac{\mu V}{\sigma} = 0.02$, Weissenberg number $Wi = \frac{\lambda \mu V}{W} = 0.02$, where *V* is the contact line velocity, λ_H is the polymer relaxation time, and *W* is half of the channel width. The Newtonian and the viscoelastic fluid has the same viscosity and the retardation-to-relaxation time ratio of the viscoelastic fluid is 0.5. Reprinted with permission from Ref. 57. Copyright 2012, Elsevier.

stress as predicted by the phase-field model.⁵⁷ The viscoelastic fluid is modeled by the Oldroyd-B model. It is obvious that the polymer stress is concentrated in the region within the distance $D = 2.5l_D$, i.e., the region with strong shear. This polymer stress pulls the interface toward the viscoelastic fluid. As a result, viscoelasticity in the advancing fluid enhances viscous bending, which is consistent with the experimental observations in Refs. 49,50. Conversely, viscoelasticity in the receding fluid reduces viscous bending. However, due to the small size of the inner region, the effect on the macroscopic flow is very limited.

Garoff and co-workers⁵⁸ performed experiments using Boger fluids consisting of high molecular-weight (HMW) polystyrene (PS) or polyisobutylene (PIB) dissolved in their respective oligomeric base fluids. Their observations suggest that the extra bending of interface comes from the solvent instead of the HMW polymer solute. This counterintuitive behavior can also be explained by the flow field as shown in Fig. 2A. The answer lies in the limited residence time of polymers in the strong shear region, which at the order of $\frac{D}{V}$. Since the polymer stress needs time to develop, the high shear region only favors relaxation times of order $\frac{D}{V}$ —the polymers with a shorter relaxation time have a low maximum polymer stress, while the polymers with a longer relaxation time does not have enough time to unravel. Thus the contact line only highlights the viscoelastic modes with a local Weissenberg number $\frac{\lambda_H V}{D} \sim 1$, which corresponds to $Wi \sim \frac{D}{W}$. For example, the contact line in Fig. 4 favors polymers with Wi at the order of 0.025. For typical experimental parameters, $V = 5 \times 10^{-6}$ m s⁻¹ and $D = 10^{-8}$ m, which corresponds to an optimal relaxation time of 0.002 s, of the same order as the relaxation times of the oligomeric PIB and PS solvents. This explains why the contact line is affected by the non-Newtonian rheology of the oligomeric solvent, not the HMW polymeric solute.

It should be noted that the actual flow field in the inner region of the contact line has not been measured due to the small length scales, and is thus not known with confidence. Thus the numerical results can only provide a plausible explanation of the experimentally observed viscoelastic effects on moving contact lines, and they should not be over-interpreted.

More phase-field work on wetting of viscoelastic fluids can be found in Refs. 59,60, where Amberg and co-workers investigated the spontaneous spreading and impact of viscoelasticity droplets. Their results confirmed that the contact line motion is enhanced by viscoelasticity. But this conclusion was drawn based on a fixed total viscosity, and thus part of this enhancement of contact line motion may be due to the reduction of solvent viscosity.

Wetting on rough surfaces

When a drop is gently deposited on a rough surface, the equilibrium state can be described by either the Wenzel⁶¹ or Cassie-Baxter⁶² model. For an intrinsically hydrophilic surface, the Wenzel state promotes wetting by reducing the apparent contact angle while the Cassie-Baxter state does the opposite. This scenario can however get complicated for a moving contact line due to pinning.

Yang et al.⁶³ used the phase-field model described in Phase-field formulation section to investigate the contact line dynamics in a capillary tube with microgrooves on the tube wall, as shown in Fig. 5A. At small enough *Ca*, the interface eventually reaches a quasi-steady state superimposed with periodic oscillation. For grooves with a small enough depth, the contact line sweeps over the rough surface with no receding fluid trapped, which corresponds to the Wenzel state. The critical depth for Wenzel to Cassie-Baxter transition is found to be a function of *b*, *W*, and the intrinsic static contact angle θ_S . As the contact line travels over the peaks and troughs of the grooves, it undergoes a stick-slip motion in the Wenzel state and a more complicated stickjump-slip motion in the Cassie-Baxter state.

In the Wenzel state, due to contact line pinning, the contact angle is enlarged as shown in Fig. 5B, opposite to the prediction by the Wenzel equation. Fig. 5C shows the time-averaged apparent contact angle as a function of the capillary number, which can be well fitted by the Cox theory. In particular the Cox curve with static contact angle $\theta_{S,eff} = 133.8^{\circ}$ and slip length $l_{s,eff} = 0.09W$ gives the best fitting. Thus the contact line dynamics on a rough surface can be approximated by that on a smooth surface with



Fig. 5 Dynamic wetting on a patterned surface. (A) Computational set up. (B) Snapshots of the interface, Ca = 0.00375. (C) Average apparent contact angle as a function of Ca. $\theta_S = 60^\circ$, $I_D = 0.001 W$, and the two fluids have equal viscosities. The microgrooves have dimensions a = b = 0.05W and d = 0.01W, and the system is under the Wenzel state. $T = \frac{tV}{a+b}$ and $Ca = \frac{\mu V}{\sigma}$, where V the average contact line velocity determined by the fixed flow rate. Adapted with permission from Ref. 63. Copyright 2018, American Institute of Physics.

substantially increased effective parameters $\theta_{S,eff}$ and $l_{s,eff}$. Further investigation reveals that $\theta_{S,eff}$ is essentially a time average of θ_S and $\theta_S + \frac{\pi}{2}$:

$$\cos \theta_{S,eff} = (1 - \alpha)\cos \theta_S + \alpha \cos\left(\theta_S + \frac{\pi}{2}\right),\tag{20}$$

where α is the fraction of the time interval that the contact line is pinned on the vertical wall of the grooves. In fact, $\theta_{S,eff}$ can be understood as the advancing contact angle on the rough surface, and $\theta_{S,eff} \gg \theta_S$ is consistent with the common understanding that systems under the Wenzel state exhibit strong CAH. The enhanced slip is probably related to the stick-slip motion of the contact line, but the exact mechanism is still unclear. It is well-known that a patterned surface may exhibit significantly enhanced slip if entrapped air bubbles are transformed into a continuous gas film by the shear flow.⁶⁴ But that slip is related to the liquid-gas viscosity ratio, which is apparently different from the large slip at a viscosity ratio of one as in Ref. 63.

Drops on an inclined wall

It is well known that, due to CAH, relatively small drops have a tendency to stick to solid surfaces even when the latter is tilted. The critical parameters for the onset of drop sliding satisfy

$$(\rho_1 - \rho_2) V_d g \sin \alpha = w \sigma (\cos \theta_R - \cos \theta_A), \tag{21}$$

where V_d is the volume of the drop, *w* is the width of the drop, *g* is the gravitational acceleration, α is the wall inclination angle, and subscripts $_1$ and $_2$ denote the drop and ambient fluids. This relation was first given by Furmidge⁶⁵ based on experimental observations, and was later proved to be exact by Dussan V. and Chow⁶⁶ as long as the footprint of the drop is convex. For a hemispherical drop with radius R_0 on an inclined wall, this relation gives a critical Bond number

$$Bo_c = \frac{\cos \theta_R - \cos \theta_A}{\frac{\pi}{3} \sin \alpha},\tag{22}$$

below which the drop sticks to the wall. Here we have used the approximation $w = 2R_0$ and the Bond number is defined as $Bo = \frac{(\rho_1 - \rho_2)gR_0^2}{\sigma}$. It should be noted, however, that the actual Bo_c may be slightly different from Eq. (22) since the drop may deform and thus change its width.

To demonstrate the capability of the CAH model as described in Contact angle hysteresis section, Yue²⁷ considered the motion of an initially hemispherical drop on an inclined wall as shown in the upper-left panel of Fig. 6. For the adopted angles $\alpha = 60^{\circ}$, $\theta_A = 120^{\circ}$, and $\theta_R = 60^{\circ}$, Eq. (22) predicts $Bo_c = 1.1027$. The drop in Fig. 6A achieves static equilibrium at $t^* = 24.52$, which confirms that the drop with $Bo < Bo_c$ sticks to the wall. It should be noted that the contact line may move slightly during the initial transient when the drop adjusts its shape. For $Bo > Bo_c$, the drop keeps sliding as shown in Fig. 6B.

The distribution of the dynamic contact angle along the contact line is given in Fig. 7. For the static drop in Fig. 7A, $\theta_D \in [60^\circ, 120^\circ]$ along the whole contact line, consistent with the pinning condition. For the sliding drop in Fig. 7B, $\theta_D > 120^\circ$ at the leading edge, $\theta_D < 60^\circ$ at the trailing edge, and $\theta_D \in [60^\circ, 120^\circ]$ along the two sides that are parallel to the sliding direction of the drop (i.e., the *x*-direction). Correspondingly, the contact line advances at the leading edge, recedes at the trailing edge, and is pinned at the two sides. It should be noted that the pinned contact lines that are parallel to the sliding direction is a well-known characteristic of steadily sliding drops with CAH.^{65,67} Thus the phase-field method is quite effective in the modeling of contact line dynamics with CAH.

Summary

In this article, we have discussed different aspects of the phase-field method for the moving contact line problem from our own experience. The phase-field formulation has two key components: the Cahn-Hilliard equation that evolves the diffuse interface and the wall energy relaxation equation that imposes the contact angle condition. Coupled with hydrodynamic equations, the phase-field model recovers the Cox theory at the macroscopic scale and the molecular kinetic theory at the microscopic scale. Furthermore, the phase-field model is equipped with an energy law which is a unique advantage among numerical methods for moving contact lines.

In the phase-field model, the contact line is moved by the Cahn-Hilliard diffusion with a diffusion length that is analogous to the slip length. Different from the slip models, the contact line region features a strong shear, which makes the phase-field model particularly attractive for wetting dynamics in non-Newtonian fluids. Limited by computational resources, however, the interfacial thickness and the diffusion length in phase-field simulations are typically several orders of magnitude greater than the physically relevant values. This is resolved by the establishment of the sharp-interface limit and a computational strategy that utilizes wall energy relaxation. By tuning the wall energy relaxation parameter, the phase-field model is able to reproduce the contact line dynamics in experiments using numerically affordable interfacial thickness and diffusion length.

Since the wall energy relaxation allows the contact line to be at non-equilibrium, the dynamic contact angle can deviate from the static angle. This makes it straightforward to incorporate contact angle hysteresis with a minimal modification of the wall potential.

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Bo = 1.98

Fig. 6 3D drops on an inclined wall under different Bond numbers. The dimensionless time $t^* = t/\sqrt{\frac{\rho_1 R_0^3}{\sigma}}$ is labeled in each snapshot. The following dimensionless parameters are adopted: wall inclination angle $\alpha = 60^\circ$, advancing angle $\theta_A = 120^\circ$, receding angle $\theta_R = 60^\circ$, density ratio $\rho_2/\rho_1 = 0.01$, viscosity ratio $\mu_2/\mu_1 = 0.01$, Cahn number $Cn = \frac{c}{R_0} = 0.02$, $S = \frac{\sqrt{M\mu_1}}{R_0} = 10^{-2}$, $\Pi = \frac{1}{\mu_1 \Gamma R_0} = 0.01$, and Ohnesorge number $Oh = \frac{\mu_1}{\sqrt{\rho_1 \sigma R_0}} = 1$. Adapted with permission from Ref. 27. Copyright 2020, Cambridge University Press.



Dynamic contact angle θ_D of drops on an inclined wall. Reprinted with permission from Ref. 27. Copyright 2020, Cambridge University Fig. 7 Press.

Beyond the applications discussed here, the wall energy relaxation can potentially be exploited to incorporate complex surface wetting properties such as anisotropic wetting on patterned surfaces.⁶⁸

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