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Precursor simulations in spreading using a multi-mesh adaptive finite element method

Yana Di [a,*], Xiao-Ping Wang [b]

[a] Institute of Computational Mathe. and Sci./Eng. Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing, China
[b] Department of Mathematics, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, China

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ABSTRACT

Using the phase-field model for immiscible two-phase flows, we have numerically investigated the wetting dynamics. The long-range van der Waals forces towards the solid, which drive the spreading of the wetting phase into the nonwetting phase, have been explicitly taken into account in the governing equations. Our continuum model uses the generalized Navier boundary condition (GNBC) to account for the fluid slipping at the solid surface. The accurate description of the molecular-scale contact-line hydrodynamics makes the numerical simulations cost too much to abide. In this work, we propose an efficient multi-mesh adaptive finite element method which approximates different components of the solution (velocity, pressure and phase variable) on different *h*-adaptive meshes because of their strongly different local behaviors. That allows us to study the early stage of spreading, wherein the precursor is initiated and developed if the van der Waals forces are strong enough. We find that there is indeed a transition in the spreading behavior across a critical value of the Hamaker constant. In particular, this critical value is noted to be the one that separates the partial wetting from complete wetting.

1. Introduction

If a small liquid drop is deposited on a solid, three interfaces come into play, and three interfacial tensions are involved: γ_{SV}, γ_{SL}, and γ, which are solid–vapor, solid–liquid, and liquid–vapor interfacial tensions, respectively. The important quantity is the spreading coefficient $S = \gamma_{SV} - \gamma_{SL} - \gamma$. The case where $S < 0$, is referred to as partial wetting: the liquid remains as a drop on the solid and reaches an equilibrium shape. For $S > 0$, the drop spontaneously spreads and tends to cover the solid surface. Such a situation is called complete wetting. When a spreading liquid completely wets a substrate it forms a very thin film and the long-range character of the molecular interactions must be taken into account. Ahead of the macroscopic front, we have seen that van der Waals (VW) forces lead to the formation of a mesoscopic precursor film [4,8]. The precursor films play a crucial role in the dynamics of the wetting of a solid surface by a liquid. However, understanding the wetting dynamics involving precursor films has not been an easy task because several distinct length scales are simultaneously presented in this truly multiscale problem: (i) behind the nominal contact line there is a macroscopic wedge of liquid advancing along the solid, (ii) ahead of the wedge there is a precursor film extending over a mesoscopic distance, and (iii) the precursor film ends at a real contact line of molecular length scale. The purpose of the present work is to investigate the early stage of spreading when the precursor is initiated and developed and the dynamics in the (molecular-scale) vicinity of the real contact line needs to be explicitly taken into account.

* Corresponding author. Tel.: +86 10 62587584; fax: +86 10 62542285.
E-mail address: yndi@lsec.cc.ac.cn (Y. Di).

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Considerable work has recently been devoted to diffuse-interface models, either in the guise of the Cahn–Hilliard model for immiscible fluids [2,7,12,13,15] or the van der Waals model for a liquid–vapor interface [11]. The interface is no longer treated as a mathematical surface of zero thickness, but is rather described by the profile of an order parameter ϕ that is constant in either phase. As a result, the Navier Stokes equation acquires an extra term involving $\nabla\phi$, which models surface tension, and an additional equation for ϕ itself closes the system. In [12], a generalized Navier boundary condition (GNBC) is proposed by Qian et al. for the moving contact line problem. By combining the GNBC with the Cahn-Hilliard diffusive interface model, they have obtained numerical results that can quantitatively reproduce the molecular dynamics simulation results.

In this paper, we will use the continuum hydrodynamic model developed in [12] to investigate the development of precursor in the early stage of spreading, driven by the attractive VW forces toward the solid. In our model, we consider a two-phase immiscible fluid on a clean, flat solid surface, with one phase (the wetting phase) attracted towards the solid by the VW forces. Since the phase-field function ϕ is to provide the interface information, it is only needed to be fully resolved around the transient layers with its area much smaller than the full computational domain. The mesh adaptive method is the most natural way to improve the numerical efficiency [17]. Meanwhile, for the Navier–Stokes equation, if the liquid film thickness is in the mesoscopic range, one can still ignore the molecular nature of the liquid and consider it as continuous. The long-range molecular interactions is then described in terms of the so-called disjoining pressure [4] (here the van der Waals interactions). When the thickness of the film becomes macroscopic, the disjoining pressure vanishes. Although both phase field and velocity field undergo rapid change across the interface and around the thin liquid film, their behaviors are quite different. A multi-mesh strategy seems necessary in order to enhance the computational efficiency. In [9], a multi-mesh *h*-adaptive algorithm was proposed which approximates different variables on different meshes. Such multi-mesh adaptive finite element methods are used successfully to simulate the dendritic growth in two- and three-dimensions [6]. Here we will extend the multi-mesh technique to solve the spreading and wetting problems, where the phase-field function ϕ, the pressure p, and the velocity $\mathbf{v}$ are solved on two different adaptive meshes according to their solution behavior.

The paper is organized as follows. In Section 2, we give a brief review of the phase-field model for the contact-line motion in immiscible two-phase flows incorporating the VW forces. In Section 3, we describe the finite element discretization and the multi-mesh adaption technique. The numerical results are presented in Section 4. The paper is concluded in Section 5 with several remarks.

2. Continuum phase-field model

The diffuse-interface model has been widely used to describe the continuum hydrodynamics in immiscible two-phase flows. In particular, it has been used to remove the contact-line stress singularity. The recent discovery of the generalized Navier boundary condition (GNBC) together with the continuum model proposed in [12] have provided an accurate description for the moving contact-line hydrodynamics in immiscible two-phase flows.

2.1. Governing equations and boundary conditions

For a sharp interface impenetrable by the flow, considering the phase-field ϕ measuring the relative concentration of the two fluid phases, the pure kinematic condition can be expressed as

$$\phi_t + \mathbf{v}\cdot\nabla\phi = 0, \tag{2.1}$$

which describes the transport of the phase field by the flow. The dynamics of ϕ in a diffuse-interface description can be relaxed (or approximated) using either the relaxational Allen–Cahn equation or the diffusive Cahn–Hillard equation. In the following, we choose to use the Allen–Cahn dynamics whose numerical treatment is simpler than that of the Cahn–Hilliard equation which involves fourth-order derivatives. It is well known that, being a continuity equation, the Cahn–Hilliard equation treats the phase field as a conserved quantity, while under the Allen–Cahn equation the phase field is not conserved. Therefore, a Lagrange multiplier is introduced to the Allen–Cahn equation to enforce the conservation of ϕ [5,10]. The modified Allen–Cahn equation reads:

$$\phi_t + \mathbf{v}\cdot\nabla\phi = -M_1[\mu + \lambda(t)], \quad \frac{d}{dt}\int_\Omega \phi dx = 0, \tag{2.2}$$

where M_1 is a positive parameter responsible for the rate of relaxation, $\mu = -K\nabla^2\phi + f'(\phi)$ is the chemical potential with $f(\phi) = -\phi^2/2 + \phi^4/4$. $\lambda(t)$ is the Lagrange multiplier, which can be derived from

$$\lambda(t) = \frac{1}{|\Omega|}\left[\int_\Omega (\phi^3 - \phi)d\Omega - \int_\Gamma \partial_n\phi d\Gamma\right]. \tag{2.3}$$

The two coupled equations of motion are the convection-diffusion equation for the phase field and the Navier–Stokes equation in the presence of the capillary force density as proposed in [12]. To facilitate the numerical computation, the governing equations and boundary conditions are non-dimensionalized, with ϕ scaled by $|\phi_\pm| = \sqrt{r/u}$, lengths by $\xi = \sqrt{K/r}$, velocity by the reference speed V_0, time by ξ/V_0, pressure/stress by $\eta V_0/\xi$, and force density by $\eta V_0/\xi^2$. The Lagrange multiplier is scaled by $K|\phi_\pm|/\xi^2$. The dimensionless equations are