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A level-set method for two-phase flows with moving contact line and insoluble surfactant

Jian-Jun Xu [a], Weiqing Ren [b,c,*]

[a] School of Mathematical Sciences, Xiangtan University, Xiangtan, Hunan, 411105, China
[b] Department of Mathematics, National University of Singapore, Singapore, 119076, Singapore
[c] Institute of High Performance Computing, Agency for Science, Technology and Research, Singapore, 138632, Singapore

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ABSTRACT

A level-set method for two-phase flows with moving contact line and insoluble surfactant is presented. The mathematical model consists of the Navier–Stokes equation for the flow field, a convection–diffusion equation for the surfactant concentration, together with the Navier boundary condition and a condition for the dynamic contact angle derived by Ren et al. (2010) [37]. The numerical method is based on the level-set continuum surface force method for two-phase flows with surfactant developed by Xu et al. (2012) [54] with some cautious treatment for the boundary conditions. The numerical method consists of three components: a flow solver for the velocity field, a solver for the surfactant concentration, and a solver for the level-set function. In the flow solver, the surface force is dealt with using the continuum surface force model. The unbalanced Young stress at the moving contact line is incorporated into the Navier boundary condition. A convergence study of the numerical method and a parametric study are presented. The influence of surfactant on the dynamics of the moving contact line is illustrated using examples. The capability of the level-set method to handle complex geometries is demonstrated by simulating a pendant drop detaching from a wall under gravity.

1. Introduction

Modeling and simulation of multi-phase flows have attracted a lot of attention in computational fluid dynamics in recent years. Main challenges in this problem arise from tracking the fluid interface, imposing the interface jump condition, large capillary force, large density/viscosity ratio, etc. Much effort has been made to address these issues and many numerical methods have been developed, among which the most popular ones include the level-set method [30,42], the front tracking method [12,49], the volume of fluid method (VOF) [17], the diffuse interface method [2], the immersed boundary method [28,31], the boundary integral method [18,32], the immersed interface method [22,24], etc.

Most of these earlier works focused on closed interfaces and/or simple fluids without surfactant. The purpose of the current work is twofold. One is to develop a numerical method for multi-phase flows with moving contact lines and surfactants. The other is to understand the influence of surfactants on the contact line dynamics. We will use the contact line model developed by Ren et al. [36,37], in which the boundary conditions consist of the Navier slip condition and a relation between the dynamic contact angle and the contact line speed. The numerical method is based on the level-set method for multi-phase flows with insoluble surfactants proposed in Refs. [51,54]. The presence of the solid wall and the moving contact line poses new challenges in the simulation. In the current work, we are mainly interested in the dynamics of the

* Corresponding author at: Department of Mathematics, National University of Singapore, Singapore, 119076, Singapore.
E-mail addresses: jjxu21@xtu.edu.cn (J.-J. Xu), matrw@nus.edu.sg (W. Ren).

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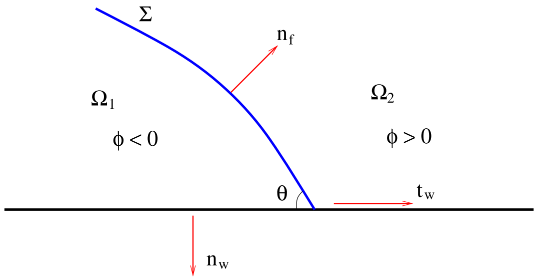

Fig. 1. Schematics of a moving contact line. Ω_1 and Ω_2 are the two fluid domains, Γ is the fluid interface, θ is the contact angle defined on the side of fluid 1, ϕ is the level-set function, $\mathbf{n}_f$ and $\mathbf{n}_w$ are the unit normal vector to the fluid interface and to the solid wall respectively, $\mathbf{t}_w$ is the unit tangent vector to the wall. $\mathbf{n}_f$ and $\mathbf{t}_w$ point from fluid 1 to fluid 2.

contact line, so we pay special attention to the implementation of the boundary conditions along the solid wall, including the boundary conditions for the velocity field and the dynamic contact angle, the boundary condition for the re-initialization equation of the level-set function, and the boundary condition for the surfactant equation.

When two immiscible fluids are placed on a substrate, the line where the fluid interface intersects the solid substrate is called the contact line (or the contact point in 2d; see Fig. 1). When one fluid displaces the other fluid, the contact line moves on the solid substrate. The phenomenon of moving contact line is pertinent to numerous industrial processes and life sciences (see e.g. [15]).

The equilibrium configuration of the static contact line is well-understood and is described by the Young's relation, which relates the three coefficients of interfacial tension to the contact angle formed by the fluid interface with the solid surface:

$$\sigma \cos\theta_Y = \sigma_2 - \sigma_1, \tag{1}$$

where θ_Y is the static contact angle, σ and $\sigma_{1,2}$ are the surface tensions of the fluid interface and the fluid–solid interfaces respectively.

The moving contact line problem, however, has for many years remained an issue of controversy and debate [10,14,5]. The main difficulty stems from the fact that classical hydrodynamic equations coupled with the conventional no-slip boundary condition predicts a singularity for the stress that results in a non-physical divergence for the energy dissipation rate [19,9]. A lot of efforts have gone into modifying the hydrodynamic model in order to remove this singularity. In most of these modified models, slip is postulated to occur near the contact line, and the contact angle is usually fixed and equal to the static contact angle. A mesh-dependent dynamic contact angle model was proposed by Afkhami et al. [1]. There the numerical method is based on Cox's analysis [8] and it aims at large-scale simulations. It uses the no-slip boundary condition in VOF simulations. It does not require resolving the slip region near the contact line but the dynamic contact angle needs to be varied according to the mesh size in order to achieve convergence.

Using principles of thermal dynamics and careful molecular dynamics studies of the physical processes near the moving contact line, Ren et al. derived a set of boundary conditions for the moving contact line problem [36–39]. This mesoscopic model consists of the Navier boundary condition for the slip velocity at the wall and a contact angle condition which relates the dynamic contact angle to the slip velocity of the contact line (see Eqs. (4) and (7) in Section 2.1). A generalized Navier boundary condition was derived using a diffuse interface approach [33,34].

The presence of surfactant can change the surface tension of the fluid interface, thus, alter the flow field and the dynamics of the fluid interface significantly. Surfactant plays a critical role in many industrial and bio-medical applications (see e.g. [16,29]). In this paper, we focus on insoluble surfactant. The molecules of insoluble surfactant have a hydrophilic head and a hydrophobic tail, thus they tend to accumulate on the fluid interface, resulting in a reduced interfacial tension. The dynamics of surfactant concentration is governed by a convection–diffusion equation on the fluid interface. It is coupled with the velocity field and changes the surface tension of the fluid interface. Solving the convection–diffusion equation on the fluid interface poses another challenge in the simulation.

Several numerical methods have been developed recently for the simulation of multi-phase flows with moving contact lines. These include the volume of fluid method [40,44,1], the front tracking method [13], the level-set method [38,25,59,45], methods using diffuse interface models [34,33], and coupled level-set and volume of fluid method [57]. More can be found in a recent review paper [46]. Few works include the effect of surfactant on contact line dynamics. A boundary integral method was used in Ref. [58] to simulate the effect of surfactant on a drop deformation on a plane wall. An immersed boundary method was developed in Ref. [21] for computing moving contact line dynamics with surfactant. In that work, the unbalanced Young stress was used as a driving force for the moving contact line and was directly included into the momentum equation for the velocity field.

A level-set method for interfacial flows with insoluble surfactant (without contact line) was proposed in Ref. [52]. The method couples the immersed interface method with an Eulerian level-set surfactant solver [51]. It was used to simulate phase separation and surfactant-laden drop–drop interactions [26,53]. The method was extended to 3D in Ref. [56]. Recently a level-set continuum surface force (CSF) method was developed in Ref. [54], which can handle problems with large viscosity