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Diffuse interface simulation of ternary fluids in contact with solid

Chun-Yu Zhang [a], Hang Ding [a,b,*], Peng Gao [a,b], Yan-Ling Wu [a]

[a] Department of Modern Mechanics, University of Science and Technology of China, Hefei 230027, China
[b] State Key Laboratory of Fire Science, University of Science and Technology of China, Hefei 230027, China

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A B S T R A C T

In this article we developed a geometrical wetting condition for diffuse-interface simulation of ternary fluid flows with moving contact lines. The wettability of the substrate in the presence of ternary fluid flows is represented by multiple contact angles, corresponding to the different material properties between the respective fluid and the substrate. Displacement of ternary fluid flows on the substrate leads to the occurrence of moving contact point, at which three moving contact lines meet. We proposed a weighted contact angle model, to replace the jump in contact angle at the contact point by a relatively smooth transition of contact angle over a region of 'diffuse contact point' of finite size. Based on this model, we extended the geometrical formulation of wetting condition for two-phase flows with moving contact lines to ternary flows with moving contact lines. Combining this wetting condition, a Navier–Stokes solver and a ternary-fluid model, we simulated two-dimensional spreading of a compound droplet on a substrate, and validated the numerical results of the drop shape at equilibrium by comparing against the analytical solution. We also checked the convergence rate of the simulation by investigating the axisymmetric drop spreading in a capillary tube. Finally, we applied the model to a variety of applications of practical importance, including impact of a circular cylinder into a pool of two layers of different fluids and sliding of a three-dimensional compound droplet in shear flows.

1. Introduction

Flows with moving contact lines (MCLs), where three different phases such as gas/liquid/solid meet, are commonly seen in nature and our daily lives, e.g. impact of an object into a water pool [1], sliding of rain drops on window panes [2] and removal of oil stain from clothes. They are also of particular importance in many industrial processes, such as film coating [3], pesticide spraying on the plant leaves etc. In the continuum assumption of fluids, stress singularity is encountered at a MCL [4], due to the incompatibility between the non-slip boundary condition at a solid wall and the physical displacement of the contact line. A variety of MCL models have thus been proposed for numerical simulation and theoretical analysis of flows with MCLs, e.g. Navier slip [5], precursor layer film [6], condensation and evaporation [7] and diffuse interface [8,9] etc. Despite their differences in the physical interpretation of contact line motion, these models effectively provide a slip at the contact line, and consequently allow it to move on the substrate. Combining MCL models

* Corresponding author at: Department of Modern Mechanics, University of Science and Technology of China, Hefei 230027, China.
E-mail address: hding@ustc.edu.cn (H. Ding).

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with interface tracking methods and Navier–Stokes solvers, one can simulate the flows with MCLs on a macroscopic scale, e.g. inertial effect in droplet spreading [10], sliding and pinch-off of droplets in shear flows [11]. More details can be found in a recent review article [12].

Numerical approaches for interface evolution of ternary fluid flows without MCLs have been modeled and extensively investigated using different interface capturing/tracking methods, such as diffuse interface [13–15], level sets [16–18], smooth particle hydrodynamics [19] and lattice Boltzmann [20]. We note that a different kind of contact line (hereinafter called triple line) also exist in ternary fluid flows, where three different fluids meet (see Fig. 1). However, the triple line is very different from the contact line among the fluids and substrate regarding the mathematical modeling. First of all, the flow motion does not encounter stress singularity at the contact line among the ternary fluids. Second, the angles between the interfaces in the ternary fluids (φ_1, φ_2 and φ_3 in Fig. 1) can be derived from the force balance of surface tensions at the contact line. In contrast, the microscale contact angle is related to the force balance in the *tangential* direction of the substrate at the contact line, i.e. the Young's equation.

Although numerical simulations of flows with MCLs and ternary fluid flows have been well developed separately, there is lack of numerical studies on ternary fluid flows with MCLs, which were found important in industrial processes such as cleanup of oil spills [21]. To develop appropriate wetting conditions at the substrate is crucial for accurate simulation of the evolution and coupling of the fluid–fluid interfaces. We note that the presence of multiple-component fluids gives rise to additional difficulties in numerical modeling and simulations compared to two-phase flows with MCLs. There exist not only MCLs among two fluids and the substrate, but also moving contact points where three MCLs meet (see Fig. 2 for an example). How to model the contact point, particularly letting the interfaces intersect the substrate at certain contact angles at this point, remains an issue. On the other hand, the wettability of the solid substrate has to be modeled by multiple contact angles, which correspond to the different material properties between the fluid and the substrate. These contact angles are supposed to be prescribed, and used in the wetting conditions at the solid substrate, to provide the boundary conditions for the evolution of the fluid–fluid interfaces. These contact angles are not mathematically independent — they are associated with each other through the surface tensions [22]; in the numerical simulation, the consistency in the evolution of multiple interfaces at the contact lines and contact points also rely heavily on the appropriate treatment of these contact angles in the implementation of wetting conditions.

Recently a few researchers initiated the numerical studies on ternary fluid flows with MCLs. Ben Said et al. [22] proposed a multi-component free-energy MCL model based on the diffuse interface approach. They simulated the evolution of a compound droplet into its equilibrium state, which was driven by chemical potential only. Since the motion of the compound droplet was not coupled with solutions of Navier–Stokes equations, it significantly limits the applicability of the model. Shi and Wang [23] extended the generalized Navier boundary condition for two-phase flows with MCLs to ternary fluid flows with MCLs. Coupling with a finite element method for solving the Navier–Stokes equations, they investigated the spreading of a two-dimensional compound droplet on a substrate.

In the present work, we developed the geometrical wetting conditions for the diffuse-interface simulation of ternary fluid flows. In particular, we proposed a weighted contact angle model, in which the jump in contact angles at the contact point is replaced by a relatively smooth transition of contact angles in the 'diffuse contact-point' region of finite size (of an order of the thickness of the diffuse interface). With the help of this model, we extend the geometrical formulation of wetting condition for two-phase flows with MCLs to ternary flows with MCLs. This treatment not only greatly facilitates the implementation of the wetting conditions involved with multiple contact angles, but also lets the order parameters that represent different interfaces vary at the substrate in a consistent manner.

In the computation we used a diffuse interface ternary-fluid model to track the interface evolution [13], and solved the Navier–Stokes equations by a finite volume method on a staggered grid [24]. Combining them with the wetting conditions, we simulated two-dimensional spreading of a compound droplet on a substrate, and validated the numerical results of the drop shape at equilibrium by comparing against the analytical solution. We checked the convergence rate of the simulation by investigating the axisymmetric drop spreading in a tube. Finally, we applied the model to a variety of applications of practical importance, including impact of a circular cylinder into a pool of two layers of different fluids and sliding of a three-dimensional compound droplet in shear flows.

2. Governing equations and numerical modeling

2.1. Diffuse interface model for ternary fluid flows

We investigate here incompressible flows of ternary immiscible fluids in the presence of moving contact lines. A ternary diffuse-interface model is adopted here [13], and the mathematically sharp interfaces between the three fluids are modeled by diffuse interfaces, which have a finite thickness of a length scale ϵ. The diffuse interfaces are represented by contours of the volume fraction of the respective fluids, $\mathbf{C}$. Provided the characteristic velocity U and length L, the evolution of $\mathbf{C}$ is governed by the dimensionless Cahn–Hilliard equations,

$$\frac{\partial \mathbf{C}}{\partial t} + \nabla \cdot (\mathbf{uC}) = \frac{1}{Pe} \nabla^2 \Psi, \tag{1}$$