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A Level Set Method for the Simulation of Moving Contact Lines in Three Dimensions

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Abstract. We propose an efficient numerical method for the simulation of the two-phase flows with moving contact lines in three dimensions. The mathematical model consists of the incompressible Navier-Stokes equations for the two immiscible fluids with the standard interface conditions, the Navier slip condition along the solid wall, and a contact angle condition (Ren et al. (2010) [28]). In the numerical method, the governing equations for the fluid dynamics are coupled with an advection equation for a level-set function. The latter models the dynamics of the fluid interface. Following the standard practice, the interface conditions are taken into account by introducing a singular force on the interface in the momentum equation. This results in a single set of governing equations in the whole fluid domain. Similarly, the contact angle condition is imposed by introducing a singular force, which acts in the normal direction of the contact line, into the Navier slip condition. The new boundary condition, which unifies the Navier slip condition and the contact angle condition, is imposed along the solid wall. The model is solved using the finite difference method. Numerical results are presented for the spreading of a droplet on both homogeneous and inhomogeneous solid walls, as well as the dynamics of a droplet on an inclined plate under gravity.

AMS subject classifications: 74F10, 65M06, 76D05, 76T10

Key words: Level set method, two-phase flow, moving contact line, dynamic contact angle, Navier boundary condition.

1 Introduction

When two immiscible fluids are placed on the solid substrate, a moving contact line (MCL) forms at the intersection of the fluid interface and the solid wall. It is well-known that the classical hydrodynamics, such as the Navier-Stokes equation with the

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no-slip boundary condition, predicts a singularity for the viscous stress at the contact line. This singularity results in a unphysical divergence of the rate of energy dissipation [15]. Much effort has been devoted to removing this singularity thus regularizing the model [3,5,7,16,18,24,25]. In most of these modified models, either slip or diffusion is postulated to occur near the MCL. In the former case, the slip is usually modeled by the Navier boundary condition, in which the shear stress is assumed to be proportional to the slip velocity; in the later case, a diffuse interface is employed to address the difficulty caused by the contact line singularity.

Based on molecular dynamics simulations and thermodynamics principles, Ren et al. proposed a set of boundary conditions for the MCL problem [26,28]. Besides the Navier boundary condition for the slip velocity, a condition for the contact angle is introduced at the MCL. When the system is at static, the contact angle of the interface satisfied the Young's equation and is determined by the three surface tension coefficients. However, when the contact line moves, the contact angle deviates from the static contact angle and the deviation depends on the contact line velocity. The condition for this dynamic contact angle proposed in [26,28] states that the unbalanced Young stress, i.e. the stress arising from the deviation of the dynamic contact angle, is balanced by the friction force at the contact line. The later is proportional to the normal velocity of the contact line. In this paper, we will use this model to simulate the contact line dynamics in three dimensions (3d).

One of the main challenges in developing the numerical method is how to impose the dynamic contact angle condition. In an earlier work [27,41], it was proposed to impose this condition through a singular force at the contact line. This approach is simple and was demonstrated to be effective in the simulation of MCLs in two spatial dimensions. In this work, we extend the method to three dimensional problems.

A number of numerical methods have been proposed for the simulation of multiphase flows with MCLs, for example, in Refs. [1,2,8,9,14,19,21,24,27,29,30,34,35,41,43,45,47–49,51,52]; more can be found in the review paper [36]. These methods generally apply different approaches to represent the fluid interface and/or different contact line conditions as well as their numerical implementations. For example, the volume of fluid method was used to deal with the moving interface in [2,29], and the contact angle condition was imposed on the gradient of the volume fraction function at the contact line. In Ref. [8], Gao and Wang considered the phase field approach and they solved the Naiver-Stokes equations with the generalized Navier boundary condition by a splitting method based on pressure Poisson equation. In Ref. [34], the level set method was used to capture the fluid interface, and a dynamic contact angle model was proposed for the contact line motion dominated either by viscous effects or inertial effects. The contact angle model is then used in the reinitialization of the level set function. Recently Zhang and Yue developed a level set method in finite element framework for the 2d MCL problem [48]. In the front-tracking method, the interface is represented by a set of markers, and the contact line position is updated according to either the fluid velocity at the con-