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A Numerical Method for Dynamic Wetting Using Mesoscopic Contact-Line Models

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Abstract. Numerical simulation of wetting or dewetting processes is challenging due to the multiscale feature of the moving contact line. This paper presents a numerical method to simulate three-dimensional wetting processes in the framework of lubrication equation and Navier slip condition. A mesoscopic model of the moving contact line is implemented with a cutoff of the computational domain at a small distance from the contact line, where boundary conditions derived from the asymptotic solution of the intermediate region are imposed. This procedure avoids the high resolution required by the local interface near the contact line and enables the adoption of physically small slip lengths. We employ a finite element method to solve the lubrication equation, combined with an arbitrary Lagrangian–Eulerian method to handle the moving boundaries. The method is validated by examining the spreading or sliding of a liquid drop on the wall. The numerical results agree with available exact solutions and approximate theories.

AMS subject classifications: 35R37, 76D45, 76D08

Key words: Moving boundary problem, moving contact line, wetting, lubrication equation.

1 Introduction

The evolution of free surfaces and contact lines in wetting processes is crucial in many industrial applications [1–5]. However, the multiscale nature of moving contact lines brings challenges to numerical simulations [6]. The movement of the contact line results from both hydrodynamics and molecular kinetics, at scales that crossover six decades of magnitude [7]. A purely hydrodynamic description with the conventional no-slip boundary condition can lead to a singularity in stress and dissipation [8]. To perform a simulation

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within the framework of hydrodynamics, one should combine the governing equation with a microscopic contact line model such as a slip boundary condition [9–11], a precursor film [12], or a diffuse interface [13]. As also supported by molecular dynamics simulations of the moving contact line problem [14], one of the most commonly used models is the Navier slip condition, in which the slip velocity at the wall is proportional to the local shear rate with a nanoscale coefficient λ known as the slip length [15, 16]. Such a small length must be resolved in simulations to obtain a mesh-convergent result, which generally requires a huge calculation cost [17]. As a compromise, previous studies often adopt a much larger slip length [18–22], which hinders quantitative comparison with experiments. Most of the full-scale simulations with physical sizes of slip lengths are for stationary problems [23–25]. Time-dependent simulations with such small slip lengths have only recently been achieved for two-dimensional wetting [26, 27].

In practice, macroscopic behaviors are of main interest in an interfacial flow with moving contact lines. To circumvent the difficulty of full-scale calculations, the macroscopic flow can be numerically obtained with the help of a mesoscopic contact line model, which involves the microscopic region near the contact line and serves as boundary conditions for the macroscopic flow [4, 28]. The central element of the model involves establishing a relationship between the interfacial slope angle at the mesoscopic scale (or the dynamic contact angle) and the speed of the contact line. Such theories have been developed based on hydrodynamics for slow contact line speeds [29, 30], where matched asymptotic analysis can be used for the situations where the macroscopic interface behaves in a quasistatic [31] or highly unsteady [32, 33] manner. These works have highlighted the presence of a mesoscopic-scale region where analytical relations can be derived. Somalinga and Bose [34] adopted Cox's theory [30] as the boundary condition in their simulations and compared the results to full-scale simulations, demonstrating good agreement for slow contact line motions. Afkhami *et al.* [20] presented a model incorporating the dynamic contact angle based on Cox's theory, which provides a method to simulate contact line problems with grid convergence. Dupont and Legendre [21] implemented the dynamic contact angle at a micrometer scale and simulated the process of drop spreading, which agrees with experiments conducted by Lavi and Marmur [35]. Sui *et al.* [6] developed a rigorous contact line model based on the works by Hocking and Rivers [31] and Cox [36] and obtained numerical results that were quantitatively validated with full-scale simulations. Solomenko *et al.* [37] generalized the method of Sui *et al.* [6] to three-dimensional geometries and simulated three-dimensional contact line problems with acceptable computational costs.

For thin-film flows, it is more popular to employ a longwave approximation, as it amounts to solving a lubrication equation for the film thickness [38] rather than the Navier–Stokes equations. To handle moving contact lines, one can adopt a slip condition or a precursor film. The slip condition is more popular in analysis, while in numerics, it can lead to moving boundaries, which should be treated with the arbitrary Lagrangian–Eulerian method [39] or other kinds of coordinate transformation [40–43]. The precursor film model does not incorporate any moving boundary and can easily