Journal of Computational Physics 294 (2015) 243–257

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A volume of fluid method for simulating fluid/fluid interfaces in contact with solid boundaries

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ARTICLE INFO

Article history:
Received 1 September 2014
Received in revised form 19 February 2015
Accepted 27 March 2015
Available online 1 April 2015

Keywords:
Thin films
Solid–liquid intermolecular
Volume of fluid method
Contact angle

ABSTRACT

In this paper, we present a novel approach to model the fluid/solid interaction forces in a direct solver of the Navier–Stokes equations based on the volume of fluid interface tracking method. The key ingredient of the model is the explicit inclusion of the fluid/solid interaction forces into the governing equations. We show that the interaction forces lead to a partial wetting condition and in particular to a natural definition of the equilibrium contact angle. We present two numerical methods to discretize the interaction forces that enter the model; these two approaches differ in complexity and convergence. To validate the computational framework, we consider the application of these models to simulate two-dimensional drops at equilibrium, as well as drop spreading. We demonstrate that the model, by including the underlying physics, captures contact line dynamics for arbitrary contact angles. More generally, the approach permits novel means to study contact lines, as well as a diverse range of phenomena that previously could not be addressed in direct simulations.

1. Introduction

The interaction of fluid/fluid interfaces with solid boundaries is of fundamental importance to a variety of wetting and dewetting phenomena. In this paper, we present a computational framework for the inclusion of a general fluid/solid interaction, treated as a temporally and spatially dependent body force, in a direct solver of the Navier–Stokes equations. This approach allows for computing fluid wetting properties (such as equilibrium contact angle) based on first principles, and without restriction to small contact angles.

Due to the complexities involved in modeling dynamics of fluids on solid substrates, a significant amount of modeling and computational work has been carried out using the long-wave (lubrication) approach. Still, even within the long-wave approach, a difficulty arises when employing the commonly used no-slip boundary condition at the fluid/solid interface: a non-integrable shear-stress singularity at the moving contact line. Simulating dynamic contact lines therefore requires additional ingredients for the model. One option is to include fluid/solid interaction forces with conjoining–disjoining terms which lead to a prewetted (often called 'precursor') layer in nominally 'dry' regions. This approach effectively removes the 'true' contact line, consequently avoiding the associated singularity [1–3]. A second approach is to relax the no-slip condition and instead assume the presence of slip at the fluid/solid interface. Both slip and disjoining pressure approaches have been

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http://dx.doi.org/10.1016/j.jcp.2015.03.051
0021-9991/

extensively used to model a variety of problems including wetting, dewetting, film breakup, and many others (see e.g. [4,5] for reviews).

While the approach based on the long-wave model has been very successful, it does include limitations inherent in its formulation: in particular, the restriction to small interfacial slopes (strictly speaking, the slopes much less than unity), and therefore small contact angles. We have shown in our earlier work [6] that, depending on the choice of flow geometry, the comparison between the solutions of the long-wave model and of the Navier–Stokes equations may be better than expected; however, still for slopes of $O(1)$, quantitative agreement disappears. Therefore, one would like to be able to consider wetting/dewetting problems by working outside of the long-wave limit, while still considering the most important physical effects such as fluid/solid interaction forces. These fluid/solid interactions are known to be crucial in determining stability properties of a fluid film; without their presence, a fluid film on a substrate is stable, since there are no forces in the model to destabilize it. In particular, for thin nanoscale films, fluid/solid interaction forces may be dominant. We note that the approaches based on the Derjaguin approximation to include the van der Waals or electrostatic interactions into the model in the form of a local pressure contribution (disjoining pressure) acting on the fluid/solid interface are derived under the assumption of a flat film [7–10]. Therefore these approaches cannot be trivially extended to the configurations involving large contact angles.

In the context of direct simulations of the Navier–Stokes equations with free interfaces, a large variety of methods are used to track the evolution of the interface. Lagrangian methods conform the computational grid to the interface (e.g. [11–13]). Eulerian methods require a separate mechanism to track the interface location; these include front tracking methods (e.g. [14]), and interface capturing methods such as volume of fluid methods and level set methods. The latter two methods easily treat topology changes, and with recent developments have been shown to be effective for simulating surface tension driven flows [15–18]. A common feature of volume of fluid methods is that contact angles are imposed geometrically, in that the angle at which the interface intersects the solid substrate is specified as a boundary condition on the interface [19–21]. Such approaches were used to model the dynamics of non-wetting drops, that could even detach from the substrate [22], as well as spreading drops [21,23,24]. The van der Waals interaction has been implemented previously in a volume of fluid based solver for the liquid/liquid interaction of colliding droplets [25], but to our knowledge has not been considered for flows involving wetting phenomena.

A variety of other computational methods have been considered in the context of wetting/dewetting. Here we mention phase-field methods that treat two fluids with a diffuse interface by means of a smooth concentration function, which typically satisfies the Cahn–Hilliard or Allen–Cahn equations, and is coupled to the Navier–Stokes equations. Jacqmin [26] describes a phase-field contact angle model that uses a wall energy to determine the value of the normal derivative of the concentration on a solid substrate. This model has been used to study contact line dynamics [27,28], and similar models have been considered in the investigation of the sharp interface limit of the diffuse interface model [29,30]. Lattice-Boltzmann methods have also treated the contact angle with a wall energy contribution [31,32]. These approaches have explained a variety of phenomena related to spreading of fluids on solid substrates, but do not consider explicitly the stabilizing and destabilizing forces between fluid and solid, as has been done via disjoining pressure within the context of the long-wave model. The liquid/solid interaction is naturally included in molecular dynamics (MD) simulations [33–35] that typically consider Lennard Jones potential between fluid and solid particles. However, MD simulations are, in general, computationally expensive, even when simulating nanoscale systems. One would like to be able to include liquid/solid interaction within the framework of a continuum model.

Here, we present a novel approach, based on a volume of fluid formulation, which includes the fluid/solid interaction forces into the governing Navier–Stokes equations, without limitations inherent in the long-wave model. This inclusion allows for arbitrary contact angles to be incorporated based on modeling the underlying physics, in contrast to conventional volume of fluid methods. The presented approach also leads to the regularization of the viscous stress since the fluid film thickness never becomes zero. Furthermore, our framework can account for additional physical effects, such as instability and breakup of thin fluid films, that would not be described if fluid/solid interaction forces were not explicitly included. We note here that while film rupture can also occur in phase-field based approaches (as in [26]), this seems to be due to the presence of a rather thick interface, and not due to the explicit inclusion of destabilizing liquid/solid interaction forces.

In the present paper we focus on formulating and discretizing the model, and on discussing issues related to convergence and accuracy. To validate our proposed numerical scheme, we consider two representative examples, involving relaxation and spreading of sessile drops with various contact angles on a substrate. These benchmark cases permit comparison of our results with well established analytical solutions for a particular flow regime. The application of the method to the study of thin film stability including dewetting will be considered in the sequel [36].

The rest of this paper is organized as follows. We describe the details of the fluid/solid interaction in Section 2. In Section 3, we describe two finite-volume methods for the discretization of the considered fluid/solid interaction forces. The presentation in these two sections applies to any generic fluids. In Section 4, we present a comparison of the two discretization methods for equilibrium and spreading drops, for a particular choice of material parameters. In Section 5, we give an overview and future outlook.