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A level-set method for large-scale simulations of three-dimensional flows with moving contact lines

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ABSTRACT

A new method is presented to perform three-dimensional simulations of two-phase flows with moving contact lines using level-set. To account for the full range of length scales involved in the physical problem under realistic conditions, without having to resolve the flow down to the smallest continuum scale, a dynamic contact angle model based on asymptotic theory is used in conjunction with the computational method. Contact-angle hysteresis is also represented in this methodology. The method is validated against simulations wherein the flow is fully resolved over all length scales, and experiments of spreading droplets and droplets sliding down an inclined substrate.

1. Introduction

Two-phase flows often involve spreading and wetting phenomena, such as in acid gas treatment with contacting devices, microfluidics, coating films, and inkjet printing (e.g., [2]). Any motion of the contact (or triple) line occurring therein poses several formidable challenges. Using a no-slip condition at the wall would result in a stress singularity at the moving contact line [33,19,13]. This has provoked consideration of the circumstances at a nanometer scale about a contact line and various models (slip, kinetic, precursor film and diffuse interface, amongst others) have been formulated for moving contact lines; for a review see [45]. The main challenge for implementation in a computational method for two-phase flows, which is the main subject of this paper, is that these models involve a large range of length scales from the scale of, for instance, the size of a droplet, down to a length scale that is nanometric, in line with the original notion that different physical behavior mostly enters close to a contact line. Despite this different physical behavior occurring only at such a small scale, the flow behavior is affected also on a much larger scale: the contact-line speed is affected, and because the interface is strongly curved unless the capillary number based on the contact-line speed is very small. It is therefore of interest to couple a computational method that does not resolve the flow all the way down to this scale with analysis that represents the unresolved flow behavior. Such an approach, referred to as a large-scale model, has been developed previously (for a review see also [49]). This includes a level-set method formulation for two-dimensional flows, discussed further below; but although straightforward extension to three dimensions is a general advantage of level-set methods, this does not hold true when such a contact-line model is included. The main aim of the present work is to develop such a model

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for three-dimensional systems with moving contact lines. We briefly review these issues and the previous computational modeling here first.

Regarding the range of length scales involved, take, for instance, a slip model (e.g., [12]), which introduces a slip length that may be nanometric (e.g., [31]). During the spreading of a droplet of radius L, unless if this is very slow, the flow and interface shape are affected significantly on a length scale $L/\ln(1/\lambda)$, where λL is the (dimensional) slip length, and the contact-line speed is affected similarly [18,6]. Thus the flow is affected over a region that is usually only an order of magnitude smaller than the drop size. Therefore, on the one hand, an ordinary discretization of a droplet without consideration of contact lines easily enters such a scale, whereas on the other hand, simulations under realistic conditions wherein such flows are resolved down to a realistic slip length (or other small length scale) are not feasible, due to the disparity in length scales. It is therefore of interest to couple the computational method with analysis that represents the unresolved flow behavior which is the large-scale modeling approach alluded to above.

If no part of the contact-line region is resolved numerically at all, the above strategy suggests to impose a relation between an apparent contact angle and the contact-line speed (for example, see [48,15,34]). Under these restrictions, no special measures are made to accommodate contact-line motion, the only effect of the physical behavior at smaller scales enters through this relation for an apparent angle. In other words, the flow corresponds to the solution for the 'outer region' in asymptotic analysis such as that of Cox [6], at a scale much larger than the region affected significantly by the contact line. This introduces some difficulties. On the one hand, the resolution should remain coarse compared to the contact-line region (wherein the interface is curved), whereas on the other hand, the overall flow should be well resolved, which can over-restrict the possible numerical resolution. Furthermore, a suitable relation for the apparent angle would be needed, whereas no universally valid model is available for any flow in an outer region.

Beyond such a limited approach, the interface shape throughout the contact-line region is required, for coupling with the computational method. For this purpose, prior asymptotic theory can be made use of. For example, the detailed theory of Cox [6] (not just his result for a sole apparent contact angle) provides a first approximation of the interface slope as a function of the local distance to the contact line, the capillary number, the viscosity ratio, and the ratio of length scales, λ. The theory is discussed, with its extensions to higher order and accounting for inertial effects, in the next section.

The approach set out above would amount to the following in the context of interface-capturing methods based on finite volumes, wherein the scalar variable is usually defined at cell centers. The flow including part of the contact-line region will be resolved numerically. In this region, the interface is strongly curved, thus for a given grid spacing, the distance between the contact line and the center of grid cells adjacent to the substrate is first estimated. This distance is then used in the theoretical relation between the interface slope at this distance and the contact-line speed, which can then be imposed through either the slope of the interface at this first grid cell, or by the contact-line speed. We thus make use of a subgrid-scale model, provided by hydrodynamic theories, to represent the unresolved part of the contact-line region.

Several such large-scale methods coupled with hydrodynamic theories have been developed previously, but mostly for two-dimensional or axisymmetrical flows, the extension to three dimensions not being straightforward. In the level-set framework, Sui and Spelt [50] simulated *axisymmetric* droplet spreading in a regime dominated by viscosity and surface tension (referred to herein as the viscous regime), and in a regime wherein inertial effects invade a significant part of the contact-line region (referred to herein as the inertial regime). They validated their large-scale simulations against direct numerical simulations (DNS, wherein the entire flow is resolved down to the smallest continuum length scale) of droplet spreading in the viscous regime performed by Sui and Spelt [51], and experiments of Ding et al. [9] on droplet spreading with inertial effects. The results of tests of numerical convergence were reassuring, thereby confirming the basic premise of this type of approach, that the results should become insensitive to how far down the contact-line region is resolved beyond a minimum requirement. In their method, Sui and Spelt [50] imposed a contact angle boundary condition from the estimated contact-line speed through the asymptotic theory; using a constant contact angle would not yield numerical convergence unless resolving the flow down to the slip length [1,50]. The extension to three dimensions of this approach is a priori not straightforward, as the coupling with the quasi-two-dimensional theory must be imposed along the direction of the contact-line speed, which is not aligned with the computational grid. The level-set method would thereby loose its advantage of being straightforwardly extended to three-dimensional flows. Specifically, the method of Sui and Spelt [50] for imposing the contact angle was based on that of Spelt [48], who made use of ghost cells and considered a linear extrapolation of the interface beyond the wall boundary to calculate the distance to the interface for each ghost cells. This is a reconstruction method; another example using interface reconstruction in the context of flows with moving contact lines is the early work of Liu et al. [28], who developed a ghost-fluid method, albeit not for a large-scale contact-line model. It appears challenging to use reconstruction techniques for the present problem of large-scale models in three-dimensional configurations, however. Indeed, if use were made of a large-scale model, knowing the current velocity field, as done in Sui and Spelt [50], then imposing the corresponding contact angle would amount for the projection of the gradient of the level-set function onto the wall boundary to be aligned with that of the current velocity. Also, the remaining part of the gradient of the level-set function would have to be consistent with the contact angle that is imposed. Furthermore, the contact-line velocity is assumed to be the projection of the fluid velocity at the first grid cell onto the substrate.

Our main aim here is to formulate a level-set method for three-dimensional flows with a large-scale model for moving contact lines that is efficient and convenient to implement, by imposing the contact line velocity knowing the current level-set function.