3D simulations of flows with moving contact lines using a diffuse interface method: a shear-driven droplet moving on a wall

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Abstract
A diffuse interface method is used to simulate two-phase flows with moving contact lines in 3D. The specific numerical issue is the validation of the method regarding the dynamics of moving contact lines in 3D. In particular, we aim to use the method to extend previous (2D and/or creeping-flow) work on shear-driven motion of a droplet on a wall to the full 3D problem, accounting for inertial effects. First, the implementation of the diffuse interface method is validated using test cases of droplet deformation in shear flow and for capillary spreading of droplets. Results are presented for shear-driven droplets moving on a wall. The diffuse interface method is used to determine an apparent contact angle in droplet spreading, which is needed in a direct comparison with analytical work. The apparent contact angle will also be used in efforts to represent the contact-line motion as a relation between an apparent contact angle and the dimensionless contact-line speed.

Introduction
Two-phase flows with moving contact lines occur in a variety of applications. The flow in one of the fluids can sometimes be ignored, for instance in coating processes, and numerical methods have been developed for these flows (e.g., Christodoulou and Scriven 1992). But in many applications, such as in shear flow past droplets or bubbles adhering to a solid surface, both fluids play an important role in the interface deformation, and such an approximation cannot be made. This class of flows occurs in, for instance, oil or grease removal in detergency (Chatterjee 2001) and the entrainment of leukemic cells from the interior of a blood vessel wall (Cao et al. 1998). A study in shear flow past droplets adhering to a wall (see Figure 1) also provides a first step towards understanding membrane emulsification. In such emulsification processes, liquid is pumped through a membrane into a crossflow of another liquid, which shears off droplets to form an emulsion (Charcosset et al. 2004)

Previous work in this area has been primarily on the creeping-flow problem, especially for cases in which the contact line is pinned (e.g., Dimitrakopoulos & Higdon 1998) such that BEM-type techniques could be used. Recently, this has been extended by us to account for inertial effects, and to use arguments from the moving-contact-line literature to represent the numerical results in analytical form (Spelt 2006). That previous work was restricted to the 2D problem. A level-set approach was used (Spelt 2005) to account for the contact lines, and a slip length formulation was adopted to eliminate the stress singularity at moving contact lines. A specific effort was made to eliminate any mass conservation errors in the level-set method, through an ad-hoc global volume correction. An example result is shown in Figure 2, wherein a moving droplet is shown together with instantaneous stream-function contours in a frame of reference moving with the contact lines. The imposed shear flow is from left to right. It is seen that the resulting flow inside the droplet is more or less a rolling motion between the two contact lines. The main result of that previous work is that apparent contact angles could be determined, and it was shown that these are related to the contact-line speed through a Cox-Voinov type expressions (Spelt 2006).
In the present work, we set out to study the corresponding 3D problem, again accounting for the effects of inertia and allowing contact lines to move. During the Colloquium we shall report on results for flows in which the contact angle is fixed at 90 degrees, such that a diffuse interface method can be used (Jacqmin 1999). This will ensure exact mass conservation, which is crucial in these flows, and the diffuse interface does not lead to a contact-line singularity. Also, it is an efficient numerical method that is also relatively easy to implement. The crucial questions to be addressed at the Colloquium are: the conditions in which droplets are (partially) entrained, and to determine the relation for the speed at which a quasi-steady droplet moves, in terms of, e.g., a macroscopic contact angle.

**Numerical method**

In the diffuse interface method the interface between different phases is represented by a smooth transition region of finite thickness. Topological changes of the diffuse interface are governed by the convective Cahn-Hilliard equation (e.g., Cahn 1958, Jacqmin 1999, 2000):

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = \nabla \cdot (M \nabla \mu)$$

where $c$ is the order parameter, $M$ the mobility and $\mu$ the chemical potential. In this equation, the interfacial diffusion fluxes are approximated as being proportional to chemical potential gradients. In the present method, we select the volume fraction as the order parameter; thus $c=0$ in one fluid, and $c=1$ in the other.

The challenging problem in numerically solving the Cahn-Hilliard equation lies in the fact that it is a nonlinear fourth-order partial differential equation. To remove the stability constraint due to the nonlinearity, we use a time-split semi-implicit discretization (Badalassi et al. 2003). Fifth-order weighted essentially non-oscillatory (WENO) scheme is employed for the spatial discretization of the convection term (Liu et al. 1994). Thus, the unphysical oscillation of the order parameter away from the interface, where convection dominates, is effectively suppressed. For the Navier-Stokes solver, the marker-and-cell (MAC) projection method is used so that the resulting velocity field on the staggered grid is divergence-free. Numerical validation of this scheme has been completed for two-dimensional droplet deformation in shear flows. The results (see Figure 3) show a good agreement with those obtained by Lee et al. (2006).

Flows with moving contact lines are simulated by specifying the particular boundary condition for the order parameter in terms of the static contact angle. In this study, we restrict the contact angle to 90 degrees, which leads to a natural boundary condition for the order parameter at the solid surface. The diffuse interface method removes the stress singularity encountered by the classical sharp interface methods, so a no-slip boundary condition is used on solid walls.
Preliminary results and discussion

In this extended abstract we present preliminary results for two 3D flows with moving contact lines. The first is capillary spreading, in which a liquid droplet spreads on a solid surface as driven by capillary force. The second case is the deformation of a droplet in a creeping shear flow. In both cases, the contour of \( c=0.5 \) is defined as the interface.

The computation of the first case is performed on a mesh of \( 201 \times 101 \times 201 \). The initial radius of the droplet is set as the unit length and the initial contact angle is set to 140 degrees. Figure 4a shows the deformed shapes of the droplet at different times. It was verified that the flow is axi-symmetrical. In the figure, we show the intersection of the interface in the \( x-y \) plane. It is clear that the interface gradually approaches its equilibrium state as time progresses. In order to quantify the results, and possibly compare these with analytical results, we have computed the maximum value of the angle that the interface makes with the horizontal. In previous work (Spelt 2005, 2006) it was found that this could be associated with the apparent contact angle in analytical work. Figure 4b presents the plot of the time evolution of this ‘apparent contact angle’. We can see that the apparent contact angle finally reaches the static value of 90 degrees. Note that these results are for identical fluids. Previous work (Spelt 2005) indicates that a density and viscosity ratios of about 20 will be sufficient to compare with analytical work that ignores the exterior fluid flow. We expect to be able to present such comparison with analytical work at the Colloquium.

A schematic of the problem set-up for a droplet moving on a wall in a shear flow is shown in Figure 1. We present here results performed on a mesh of \( 201 \times 51 \times 101 \), which corresponds to a domain of \( 4L \times L \times 2L \). A uniform shear flow and a spherical cap droplet shape are imposed as the initial conditions. The non-dimensional flow parameters are set as follows: capillary number \( \text{Ca} (= \mu U / \sigma) = 0.14 \) and Reynolds
number $Re \left( = \frac{\rho U L}{\mu} \right) = 2$, where $U$ is the top-wall velocity and $L$ is the height of the channel. The initial radius of the droplet is set to $0.33L$. Some preliminary results have been obtained. For example, the shape of the moving droplet is shown in Figure 5b and a dash-dot-dot circle is superimposed for a comparison.

![Figure 5. Moving droplet in a shear flow: a droplet shape, b contact line shape.](image)

Additional results will be presented at the Colloquium, especially including results for a range of values of Ca and Re that show under what circumstances droplets are (partially) entrained by the shear flow. Also, results will be presented for apparent contact angles as a function of the capillary number based on the contact-line speed. Possible limitations of the diffuse interface method with regards to the simulation of effects of contact-line hysteresis and non-90 degree contact angles will also be discussed at the Colloquium.

References


