# Simulation of filling of microfluidic devices using a coarse-grained continuum contact angle model

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## ABSTRACT

For the design and development of new microfluidic devices reliable modelling and simulation tools must be made available. Many extensions to conventional computational fluid dynamics are required, especially multiphase fluid dynamics simulation capability. A new dynamic contact angle model is presented here, which does not require the specification of a contact angle or contact–line velocity. The level-set method is used for interface capture. The model is tested for unit problems such as relaxation to equilibrium of a contact line. It is then applied to the problem of fluid filling in a prototypical microdevice to show its utility as a design tool.

***Keywords***: contact angle, multiphase, level-set

## 1 INTRODUCTION

Microfluidic technologies have developed rapidly over the past few years. However, mature design support, in terms of modelling and simulation tools, is yet largely unavailable. In particular, many extensions to conventional computational fluid dynamics (CFD) are required: small scale physical effects such as surface forces, dynamics of three–phase contact lines, heterogeneous chemical reactions, surfactants, etc. are some obvious examples.

Incompressible two-phase flows with moving contact lines are common in a variety of applications, such as coating and biological processes. One of the difficulties in simulating such flows is that the NavierStokes equations for both fluids, in combination with no-slip boundary conditions, predict a shear stress singularity at the contact line. Also, the contact angle made by the interface with the solid surface needs to be specified. Several attempts have been made in the past decades to model contact–line dynamics within the continuum fluid dynamics framework. Generally, models are used where contact angles are prescribed based on front velocities and criteria for advancing and receding scenarios[1]. However, these models do not take into account the physical forces acting in the triple line region.

The model presented in this study is based on the molecular dynamics[2] description of the contact–line. such that it does not require the specification of contact angles. Instead of specifying the contact angle a force is added to the momentum equations which is based on the Young's law and is referred to as the unbalanced Young force[3]. The stress singularity at the contact line is regularized using a slip length and integrating the logarithmic singularity upto the slip length.

The model is compared to unit simulations presented by Spelt[1]. It is then used to analyse the filling of a prototypical microdevice with liquids with different surface properties. Bubble entrapment is an common problem in the design of microfluidic devices. Occurrence of these bubbles can be avoided through careful design of the device geometry, control of the filling process, and selection of material properties (hydrophobic or hydrophilic). A reliable simulation tool can be used to make design modifications to the geometry to make sure that the design is acceptable.

## 2 SIMULATION FRAMEWORK

### 2.1 TransAT© Microfluidics Code

The code TransAT[4] is a multi–physics finite-volume code, solving multi–fluid Navier-Stokes equations. The one-fluid formulation on which TransAT is built is such that a two–fluid flow is viewed as a single fluid having material properties varying according to a colour function which distinguishes the boundary or interface between the two fluids. Specifically, both the Level-Set and the VOF Interface Tracking Methods (ITM) can be employed to track evolving interfaces.

### 2.2 Interface Tracking Context

When the exact shape of the interfaces separating two fluids is not known, or not relevant, one may resort to the averaged Two-Fluid approach, where separate conservation equations are required for each phase with appropriate interfacial exchange forces. ITMs may be invoked when the identification of interfaces needs to be precise, as in the breakup of large bubbles, droplets or liquid jets. The key to these methods is the use of a single-fluid set of conservation equations with variable material properties and surface forces. The concept is attractive, since it offers the prospect of a more subtle strategy than that offered by the two-fluid formalism, while minimizing modelling assumptions.

## 2.3 Transport Equations

The incompressible fluid dynamics equations expressed within the single-fluid formalism take the following form,

$$\frac{\partial u_j}{\partial x_j} = 0 \quad (1)$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} - \frac{\partial \sigma_{ij}}{\partial x_j} = b_i + s_i + c_i \quad (2)$$

where the RHS terms in the momentum equation (Eq. 2) represent the body forces, the surface tension expressed by Eq. 4 below, and its contact–line wall contribution, respectively. In Eqs. 1-2, where phase change is not accounted for, $\sigma_{ij}$ is the Newtonian stress tensor.

In the level-set method the interface between two fluids is represented by a continuous function $\phi$, representing the distance to the interface that is positive on one side and negative on the other. This way, both fluids are identified, and the location of the physical interface is associated with the zero level. The level-set evolution equation is given by

$$\frac{\partial \phi}{\partial t} + u_j \frac{\partial \phi}{\partial x_j} = 0 \quad (3)$$

Material properties such as the density and viscosity are updated locally based on $\phi$ and smoothed across the interface using a modified Heaviside function. Further, the fact that $\phi$ is a continuous function across the interface helps determine the normal vector $n_i$ to the interface, and thereby the surface curvature required for the definition of the surface tension,

$$s_i = \gamma \kappa n_i \delta^I(\phi) \quad (4)$$

where $\gamma$ is the surface tension of the fluid pair, *kappa* is the interfacial curvature, $\delta^I$ is a smoothed Dirac delta function centered at the interface. The level set function ceases to be a signed distance from the interface after a single advection step of Eq. 3. To restore its correct distribution near the interface, a re-distancing problem has to be solved, in which the equation below has to be integrated to steady state:

$$\frac{\partial d}{\partial \tau} - sgn(d_0)(1 - |\nabla d|) = 0 \quad (5)$$
$$d_0(\mathbf{x}, t) = \phi(\mathbf{x}, t)$$

where $sgn(x)$ is the Signum function. In TransAT Eq. (6) is solved after each advection step of Eq. (3) using the non-oscillatory (WENO) $3^{rd}$ order scheme.

## 2.4 Dynamic Contact Angle Model

The present work proposes a method for the numerical treatment of wetting dynamics based on the physical forces associated with triple lines[5]. A triple line force included in the momentum equation; this extended momentum equation could then provide a physically adequate description of wetting dynamics, eliminating the need for any particular boundary condition specifying the contact angle. The triple line force used in the present work is based on a consideration of interfacial free energy. Accordingly, it contains only two parameters: the interfacial tension between the fluids $\gamma$ and the equilibrium contact angle $\theta_{eq}$.

$$c_i = \gamma(\cos(\theta_{eq}) - \cos(\theta_{dy}))\delta_t b \quad (6)$$

where $\theta_{dy}$ is the instantaneous dynamic contact angle, $\delta_t$ is a Dirac delta function vanishing everywhere except on triple lines, with the property that for any volume $V$, the integral $\int_V \delta_t dV$ is equal to the length of the triple line segment contained in $V$, and $b$ is the unit vector normal to the triple line and parallel to the wall surface. The triple line force, is obtained by considerations similar to the derivation of Youngs Law and can be referred to as the unbalanced Young force[3].

The second issue to be dealt with for a successful simulation method for contact line dynamics is the resolution of the stress singularity that arises due to the no–slip boundary condition. In the current model, the shear stress is assumed to have a logarithmic profile as it nears the contact line[2]. At distances less than a slip length from the contact line, full slip is assumed. In the finite volume containing the contact line, the integrated shear stress is applied. The slip length is taken to be a small value $\approx 10^{-9}$.

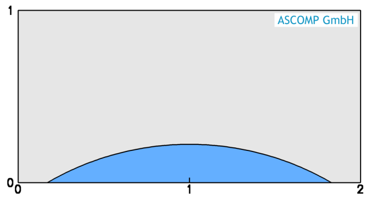
## 2.5 Numerical Details

The Navier-Stokes transport equations and the level set advection function are solved using the 3rd order Runge-Kutta explicit scheme for time integration of all variables. The convective fluxes are discretised using the 3rd order Quick scheme bounded using a TVD limiter. The diffusive fluxes are differenced using a 2nd order central scheme.

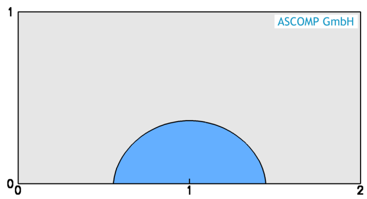
# 3 RESULTS

## 3.1 Relaxation to Equilibrium

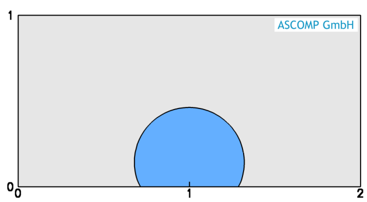
We consider here two cases presented by Spelt[1] of a droplet that is immersed in a different fluid, and adhering to a long boundary of a rectangular domain ($2 \times 1$, discretised by $2N \times N$). The fluid properties used in these cases are listed in Table 1. In Case I, the densities are equal ($= 1$) whereas the viscosities differ (droplet $4.95 \times 10^{-2}$, surrounding phase $4.95 \times 10^{-3}$). A density




(a) $t = 0s$




(b) $t = 3.7s$




(c) $t = 19.8s$

Figure 1: Return to equilibrium of a nonwetting liquid; $\theta_{eq} = 120^o$

contrast is used in Case II (droplet 1 and surrounding fluid 20) however, with constant viscosity $4.95 \times 10^{-2}$. The surface tension was chosen to be $\gamma = 0.11$ and 2.21 for the two cases, respectively and the simulations were performed for a mesh size of $128x64$.

To begin with the droplets are circular caps (radius 1.66), with contact angles being $30^o$ and $150^o$ for the dark phase (blue in Figs. 1 and 3), which is different from the equilibrium contact angles $\theta_{eq} = 120^o$ and $60^o$, respectively. The main difference of the current model from the model of Spelt[1] is that the latter case requires the additional specification of a contact–line velocity.

Figures 1 and 3 show the return to equilibrium for Cases I & II, respectively. The variation of the contact angles as the flow evolves to equilibrium is shown in Fig. 2. In Case II a faster return to equilibrium is seen driven by the higher surface tension along with an overshoot due to the higher density of the outer phase.

## 3.2 Filling of microfluidic device

With a view to show the utility of such a simulation software in practical applications, the liquid filling a prototypical microdevice like micropumps has been

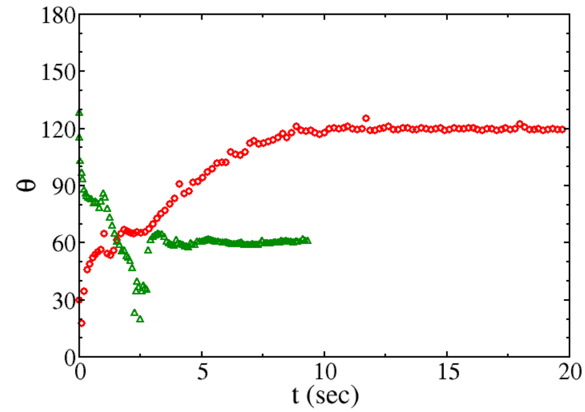



Figure 2: Variation of contact angle with time. Legend: circle - Case I; triangle - Case II.

simulated for three different liquids with $\theta_{eq} = 70^o, 90^o$ and $110^o$. Figure 4 shows the final result which shows that for the hydrophobic case special care must be taken to come up with a design which has no bubble entrapment.

## 4 Summary

A new dynamic contact angle model has been presented, which through the use of a force in the momentum equation does away with the requirement of specifying the contact angle or a contact–line velocity. Simulations were performed for the return to equilibrium of droplets and compared to other available data. Simulation of filling of a microdevice by liquids with different wetting characteristics showed that such modelling can be a useful design tool.

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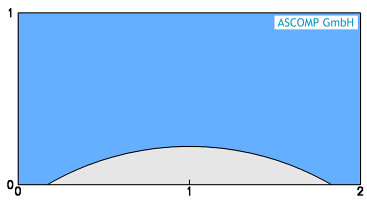
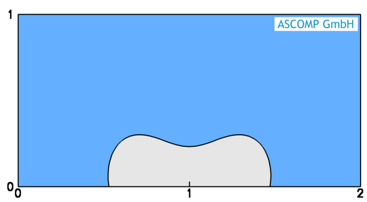
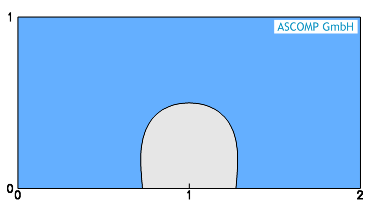


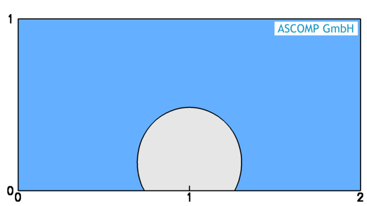

(a) $t = 0s$




(b) $t = 0.6s$

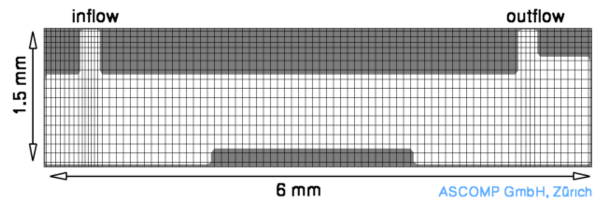



(c) $t = 1.0s$

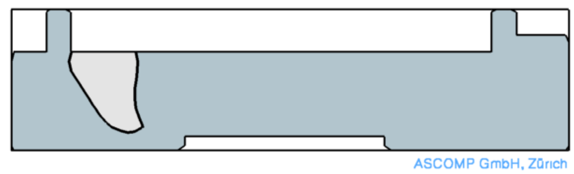



(d) $t = 3.6s$

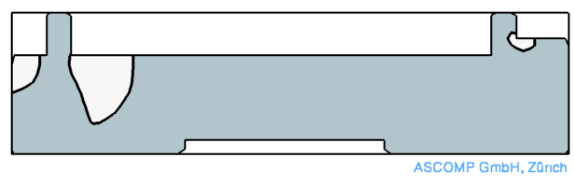
Figure 3: Return to equilibrium of a wetting liquid; $\theta_{eq} = 60^o$



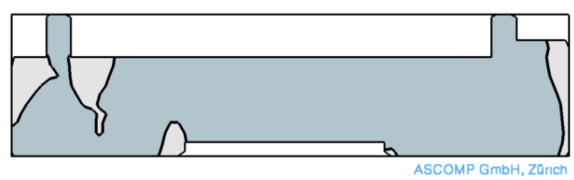

(a) Geometry and mesh




(b) Wetting $\theta_{eq} = 70^o$




(c) Neutral $\theta_{eq} = 90^o$




(d) Non-wetting $\theta_{eq} = 110^o$

Figure 4: Liquid filling of a prototype microdevice; Legend: blue - liquid, grey - air, solid line - interface, white - solid region.