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Numerical Simulation of Three-Phase Contact Lines

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Introduction

In most of the multiphase systems that involve more than two phases, contact regions appear. In the contact-line regions three phases are in mutual interaction, which can have a influence on the hydrodynamics. Depending on the phases that are in contact two general types of contact line exist: liquid-fluid-liquid and liquid-fluid-solid, see figure 1. The contact lines are usually modelled by ad hoc boundary condition for the values of the dynamic contact angles, [1].

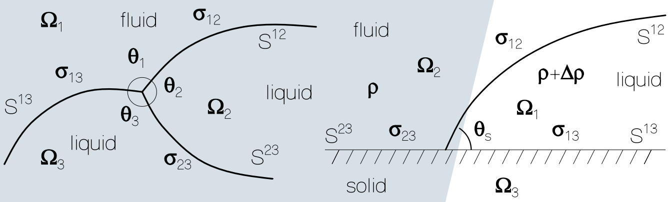

Fig. 1 *Schematic sketch of three-phase contact line: liquid-fluid-liquid type (left); liquid-fluid-solid type (right).*

Objective

To develop a computational model for a 3D simulation of multiphase flows that involve three-phase contact lines.

Mathematical method

The mathematical model is based on the assumptions that inertia is negligible and interfaces are pure (no surfactant). The main elements of the model are:

☐ Stokes equations in all liquid regions;
☐ continuity of the velocity across the interfaces;
☐ contact-line model based on a force balance in a contact-line vicinity, [2], which is rewritten in terms of capillary pressure, [3];
☐ slip condition on the solid wall in the case of liquid-fluid-solid case;
☐ normal stress balance on the interfaces which takes into account the capillary as well as disjoining pressure;
☐ the evolution is governed by the kinematic condition.

An important feature of the present model is that the values of the dynamic contact angles are not input parameters for the problem, but are part of the solution.

Numerical method

The numerical method is based on a standard boundary integral formulation, extended with the following features, [3]:

☐ non-singular contour integration of the singular layer potentials, which improves the accuracy;
☐ implementation of three-phase contact line boundary conditions and the slip condition in the liquid-fluid-solid case;
☐ multiple step integration which improves the numerical stability and increases the performance.

Results

An example of the liquid-fluid-liquid case is so called 'drop engulfing' process, figure 2, during which one of the phases can be partially or completely covered by the other.

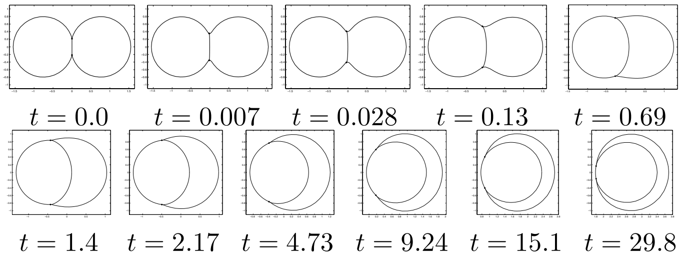
$t = 0.0$ $t = 0.007$ $t = 0.028$ $t = 0.13$ $t = 0.69$
$t = 1.4$ $t = 2.17$ $t = 4.73$ $t = 9.24$ $t = 15.1$ $t = 29.8$

Figure 2 *The compound drop evolution at* $0.5\sigma_{12} = \sigma_{13} = \sigma_{23}$.

The liquid-fluid-solid contact lines are important for processes as wetting and dewetting. Figure 3 shows detachment of a pendant drop from a plane horizontal wall.

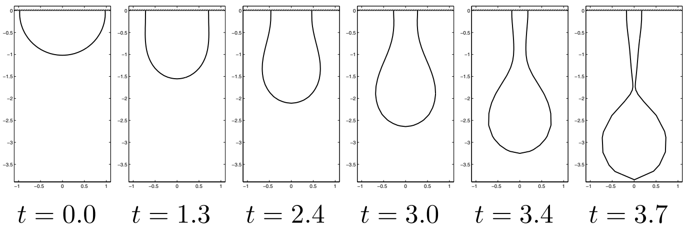
$t = 0.0$ $t = 1.3$ $t = 2.4$ $t = 3.0$ $t = 3.4$ $t = 3.7$

Figure 3 *Time evolution of a pendant drop from a horizontal solid wall at* $\sigma_{13} = \sigma_{23}$ *and* $Bo = (\Delta\rho R^2 g)/\sigma_{12} = 2$.

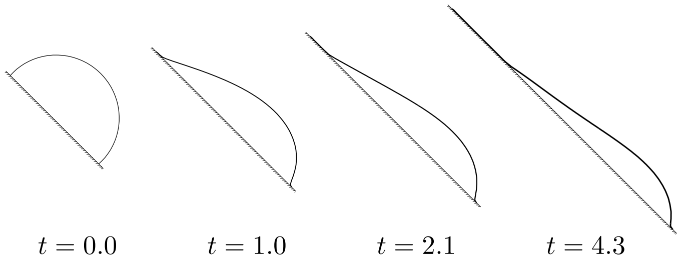
$t = 0.0$ $t = 1.0$ $t = 2.1$ $t = 4.3$

Figure 4 *The evolution of a spreading drop on an inclined at* 45^o *solid wall for* $\sigma_{23} - \sigma_{13} = \sigma_{12}$ *and* $Bo = (\Delta\rho R^2 g)/\sigma_{12} = 2$.

In the case when $\sigma_{23} - \sigma_{13} \geq \sigma_{12}$ one of the liquids completely wet the solid surface, then van der Waals forces play an important role and so called 'precursor' film is formed. In figure 4 an example of drop sliding due to gravity is shown.

Conclusions

A computational model is developed for simulation of dynamic contact-line problems. The contact line boundary conditions express force balance on a vicinity of the contact line in terms of capillary pressure, which allows straightforward incorporation in the boundary-integral method.

References:

[1] Shikhmurzaev, Y.: *J. Fluid Mech.* 334 (1997) 211–249
[2] Bazhlekov, I. and Shopov, P.: *J. Fluid Mech.* 352 (1997) 113–133
[3] Bazhlekov, I.: Ph.D. thesis, Eindhoven University of Technology (2003)