

Numerical Modelling of Two-Phase Flows with Moving Contact Lines

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Abstract

Numerical simulation is employed to simulate two-phase flow phenomena using the continuum method for surface tension modeling. The set of equations are based on the 'one-fluid' Arbitrary Lagrangian-Eulerian (ALE) description of the Navier-Stokes equations. These equations are discretized by the Finite Element method on an unstructured mesh in which the phase boundary is represented by a set of interconnected elements that are part of the computational mesh, thus a sharp representation is successfully achieved. The presented modeling will then be used to investigate two-phase flows with moving contact lines, slug and annular flows in microchannels. These problems are of great interest for technology applications such as the cooling of microelectronic devices. The employed formulation, the interface representation, bubble-wall modeling and some initial results of this Ph.D. thesis will be presented for 2-dimensional cartesian and axisymmetric cylindrical coordinates.

1 Introduction

Flows with two unmixable fluid phases are commonly found in many practical applications, such as in refrigeration industry or in cooling systems of the next generation of microelectronic devices. In the latter small scales make quantitative experimental data difficult to obtain. Numerical simulations offer an alternative approach, complementing the experimental and theoretical ones. A well established method to model fluid flow with different phases computationally is the so called one fluid formulation, where a single set of equations is used to describe the entire flow field. The effects of surface tension, which

occur only at the interface between two fluids can be modelled by a volume force as proposed by [?]. Different approaches exist to describe the motion of the interface. Eulerian methods where the computational mesh is fixed and the interface is described by the advection of a scalar field. Lagrangian methods which use a mesh moving with the flow. In this work a one fluid formulation is employed and the interface is tracked in a Lagrangian way.

Contact lines may appear in two-phase flows whenever an interface intersects with a solid boundary. Such as when a drop of liquid is placed on a surface under the influence of gravitational field. Despite its occurrence in many important applications and in everyday life contact line motion is still not physically understood.

2 Governing Equations

The Navier-Stokes equations for two-phase flow in 2d cartesian ($m = 0$) or axisymmetric cylindrical coordinates ($m = 1$) read

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_r}{\partial r} + m \frac{v_r}{r} = 0,$$

$$\begin{aligned} \rho \frac{Dv_x}{Dt} &= -\frac{\partial p}{\partial x} + \mu \Delta v_x + \rho g + f_x, \\ \rho \frac{Dv_r}{Dt} &= -\frac{\partial p}{\partial r} + \mu \left(\Delta v_r - m \frac{v_r}{r^2} \right) + f_r. \end{aligned}$$

Use has been made of the operator

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial r^2} + \frac{m}{r} \frac{\partial}{\partial r}.$$

To not interfere with the symmetry it has been assumed that gravity acts only in the direction of the symmetry axis (x -direction). The body force term

$\mathbf{f} = (f_x, f_r)^T$ accounts for the effects of surface tension modeled by [?]]

$$\mathbf{f} = \sigma \kappa \mathbf{n} \delta$$

where σ is the surface tension coefficient and δ is the Dirac distribution with support on the interface. The normal vector \mathbf{n} and the mean curvature κ are defined by the geometry of the interface. The curvature is computed by

$$\kappa_{axi} = \kappa_{2d} + m \frac{\sin(\phi)}{r}$$

where κ_{2d} is the curvature of the interface in the 2d-plane and ϕ is the angle of the interface normal relative to the symmetry axis, see Fig ??.

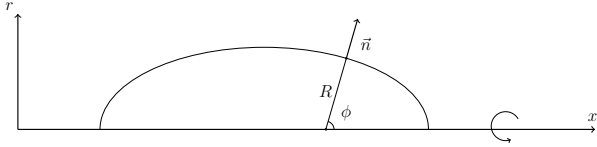


Figure 1: Axisymmetric problem formulation.

3 Mesh Description

In this work an arbitrary Lagrangian Eulerian (ALE) method is employed. This method combines the Lagrangian description (moving mesh) with the Eulerian description (fixed mesh). It makes use of boundary-adapted grids, where the mesh nodes at the interphase are moved along with the flow velocity in Lagrangian fashion while the boundary nodes remain fixed in Eulerian fashion. To ensure a good quality mesh at any time, points can be deleted, added and displaced to the mesh and the solution interpolated on the new mesh. More details regarding the computational method can be found in [?].

4 Results

In this section we describe a numerical approach to moving contact lines, which consists in imposing a

static (constant) contact angle at the three phase contact line. Such an approach is widely used in literature, see e.g. [?]. The model problem consists in a liquid drop released on a surface and surrounded by a lighter liquid or a gas. The flow is modelled in the 2d (cartesian) plane. At the beginning the drop is half-circular and a fixed value of the contact angle θ is imposed at all times. The drop deforms due to gravity which is directed downward and also as a consequence of the imposed contact angle. At steady state, the shape of the drop is given by the balance of two forces: the gravitational force which tries to spread the drop on the surface minimizing its potential energy and the surface tension which tries to minimize the drop's surface. The ratio of these two forces is described by the Eotwos number

$$Eo = \frac{\rho_l g R_0^2}{\sigma}$$

based on the initial radius R_0 of the drop and the density of the liquid ρ_l . In the absence of gravity, that is for $Eo = 0$, the drop's shape at steady state is a circular-cap. The simulation results for a case dominated by gravity ($Eo = 10$), with an imposed contact angle of 50° , can be seen in Fig. ??.

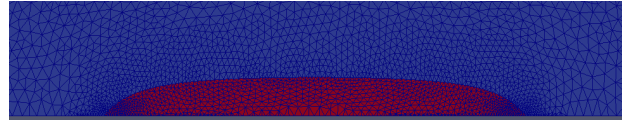


Figure 2: Final bubble shape for $Eo = 10$ and $\theta = 50^\circ$.

5 Conclusions and Further Work

In this article a numerical framework for axisymmetric simulations and static contact angles has been presented. Validations of the already implemented features namely static contact angle, phase change, annular flows will be performed. Afterwards, additional phenomena such as dynamic contact angles and Navier-Slip boundaries will also be developed.