WETTING PHENOMENA WITH ALE INTERFACE TRACKING

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Introduction

Multiphase flows are present in numerous situations in our daily live, may it be the droplet on a window while it is raining, or the liquids that we drink. They are relevant in a wide variety of industrial processes e.g. rain drops on the windshield of a car or a drop of blood in a micro fluidic device.
Within such applications, only few situations arise where there is no relevant interaction with a solid boundary as e.g. with free flow of a bubble in a column reactor. In most devices, wall boundaries are a relevant factor, as these may e.g. give the shape of the product or can cause undesired inclusions reducing the product's quality and mechanical stability. Consequently, it is crucial to provide CFD tools that can be used within the development process of products that deal with wetting phenomena in their application or during their production.
Multiphase flow phenomena on the drop or bubble scale are usually modeled via a continuum mechanical approach which is followed in this work. Here, an incompressible, immiscible, Newtonian fluid with constant fluid properties in each phase is considered. In this work, the multiphase flow is modeled as a free surface flow, where the gaseous phase is neglected. Additionally, Marangoni effects are neglected. This leads to solving the Navier-Stokes equations in combination with the mass and momentum transmission conditions at liquid free surface on a deforming domain $\Omega_-(t)$. In addition to the constitutive equation for the Cauchy stresses $\mathbf{S}$ and a relation for the dynamic contact angle is required. As boundary conditions on the wall, a generalized slip boundary condition with slip coefficient β is assumed. This yields the following analytical model:

Mass & momentum conservation
for $t > 0,\ x \in \Omega_\pm(t)$

$$\operatorname{div}\mathbf{v} = 0$$
$$\rho\partial_t\mathbf{v} + \rho\operatorname{div}(\mathbf{v}\otimes\mathbf{v}) = \operatorname{div}\mathbf{S} + \rho\mathbf{g}$$

Boundary conditions
for $t > 0,\ x \in \mathcal{S}(t)$

$$\mathbf{v}\cdot\mathbf{n}_\mathcal{S} = 0$$
$$\mathbf{P}_\mathcal{S}\mathbf{v} + \beta\mathbf{P}_\mathcal{S}\mathbf{S}\mathbf{n}_\mathcal{S} = 0$$

Mass & momentum transmission
for $t > 0,\ x \in \Sigma(t)$

$$[\![\mathbf{v}]\!] = 0$$
$$-[\![\mathbf{S}]\!]\mathbf{n}_\Sigma = \sigma\kappa\mathbf{n}_\Sigma$$

Constitutive equations

$$\mathbf{S} = -p\mathbf{I} + \mu(\nabla\mathbf{v} + \nabla\mathbf{v}^\mathrm{T})$$
$$\theta = f(\mathrm{Ca}), \quad \mathrm{Ca} = \mu v_\Gamma/\sigma$$

Jump brackets:
$$[\![\phi]\!] := \lim_{h\to 0}(\phi(\mathbf{x}_\Sigma + h\mathbf{n}_\Sigma) - \phi(\mathbf{x}_\Sigma - h\mathbf{n}_\Sigma))$$

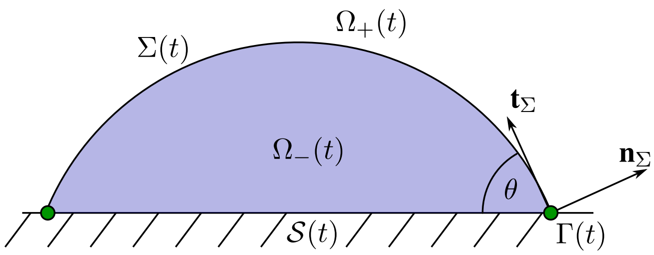

Figure 1: Illustration of bulk phases for the gaseous and liquid phases $\Omega_+(t)$ and $\Omega_-(t)$ that are separated by the liquid gas interface $\Sigma(t)$. The droplet wets a planar solid wall on the area $\mathcal{S}(t)$ and forms a contact line $\Gamma(t)$ where surface normal and tangent vectors $\mathbf{n}_\Sigma$ and $\mathbf{t}_\Sigma$ are depicted. As the domain changes over time, all illustrated quantities depend on time t.

Here, μ and ρ are the dynamic viscosity and density of the liquid, v_Γ is the contact line velocity, κ is twice the mean curvature of the free surface, σ is the surface tension coefficient, $\mathbf{g}$ is the vector of gravitational acceleration, and Ca is the capillary number. The relevant sets are the gaseous and liquid phases $\Omega_-(t)$ and $\Omega_+(t)$, the interface $\Sigma(t)$, the contact line $\Gamma(t)$ and wetted wall $\mathcal{S}(t)$, all illustrated in figure 1. Furthermore, $\mathbf{P}_\mathcal{S}$ is the projector onto the wall boundary.
While multiphase flows are undoubtedly relevant in various phenomena in nature and industry, it is still under debate what models are needed to resolve certain hydrodynamic phenomena. Simpler models are of the form $\theta = f(\mathrm{Ca})$. In the simplest way, the contact angle is modeled constant or via a advancing and receding contact angle. Experimental results can provide a functional relation, e.g. [1, 2, 3]. More sophisticated models e.g. [4] addresses the moving contact line paradox, see [5] however, they require the solution of coupled partial differential equations on the boundaries of the moving liquid domain.

ALE - Interface Tracking

The wetting problem described above is solved with OpenFOAM's arbitrary Lagrangian Eulerian (ALE) interface tracking method [6, 7]. With this approach a subset of the mesh boundary coincides with the interface allowing to accurately track its deformation. This means that when the interface is moving, the interface mesh is following this change. Aiming for mass conservation, the interface is moved using a control-point based algorithm [8]. To maintain overall mesh quality, the bulk mesh has to adapt to this deformation by mesh motion (controlled by mesh modifiers) or remeshing. While the effort to move the mesh is extensive and does also limit the capability to capture highly deforming domains without remeshing, it provides a consistent surface mesh. This outstanding feature of the interface tracking method can be used to simulate the evolution of surface active species (surfactants) usually present on the liquid gas interface by means of a finite area method. This is an important feature to model actual physical systems, as even a small contaminations by surfactants can significantly influence the surface tension coefficient and thereby the hydrodynamics of flow [9, 10, 11].

Results

The ALE interface tracking method has been extended to handle wetting phenomena and provides a library for dynamic contact angle models. Boundary conditions have been added to allow the simulation of wetting of planar surfaces. These simulations include among others the verification case where a drop is spreading on a planar surface for varying Eötvös numbers. A more complex validation is performed by comparison to experimental data. This allows to compare results for varying wall boundary conditions where the contact line of a drop with increasing volume is modeled.

Stationary Droplet

To validate the wetting models that have been implemented into the existing ALE interface tracking framework, the test from [12] is used. This setup can be used in 2D or 3D and consists of a droplet that is initialized as e.g. a hemisphere. Then, the simulation is started to obtain the stationary state of the system. When varying the Eötvös number e.g. by varying the magnitude of the gravitational acceleration, the stationary state of the drop is flattening with increasing Eötvös number. Analytic reference solutions are available for one regime where gravitation is the dominant effect and the other where surface tension is the relevant influence on the drop shape. In addition simulation results from a volume of fluid approach are available for the full spectrum of Eötvös numbers including the transition region between the two regimes mentioned before. Results for this test case are given in figure 2. It can be seen that the ALE simulation results show an overall excellent agreement with the analytic reference solutions as much as with the simulation results from [12].

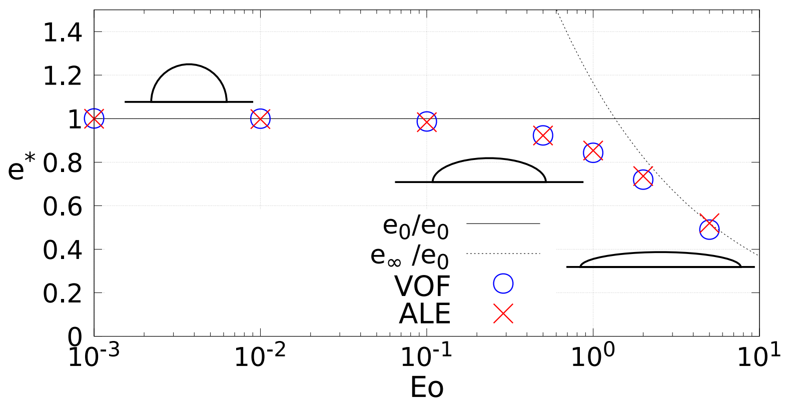

Figure 2: Comparison of non-dimensional stationary drop height e^* over varying Eötvös numbers. The straight horizontal line at $e^* = 1$ shows the limit vanishing Eötvös number. The dotted line indicates the limiting case for a gravity dominated regime. Reference data from a volume of fluid method (VOF) obtained from [12] is (blue circles) compared to ALE interface tracking results from OpenFOAM (red crosses).

Growing Droplet

In order to evaluate the implemented wetting model in comparison to experimental data, a spherical cap shaped drop is initialized. Here, the initial contact angle depends on the equilibrium contact angle of the fluid-surface combination. To achieve a moving contact line situation, liquid is pumped into the droplet from an opening on the surface. This setup is illustrated in figure 3. It shows the clipped region of a liquid drop on a planar surface. The colored mesh indicates the magnitude of the velocity inside the liquid bulk phase. The light blue stream lines illustrate the inflow of liquid from the bottom. The inflow region can be identified by a higher velocity magnitude marked in red. A coarse mesh is shown to illustrate the structure of the mesh. Here, a constant contact angle model with $\theta = 70°$ is used. This experimental setup allows to compare a variety of properties such as e.g. interface shape, dynamic contact angles, etc.

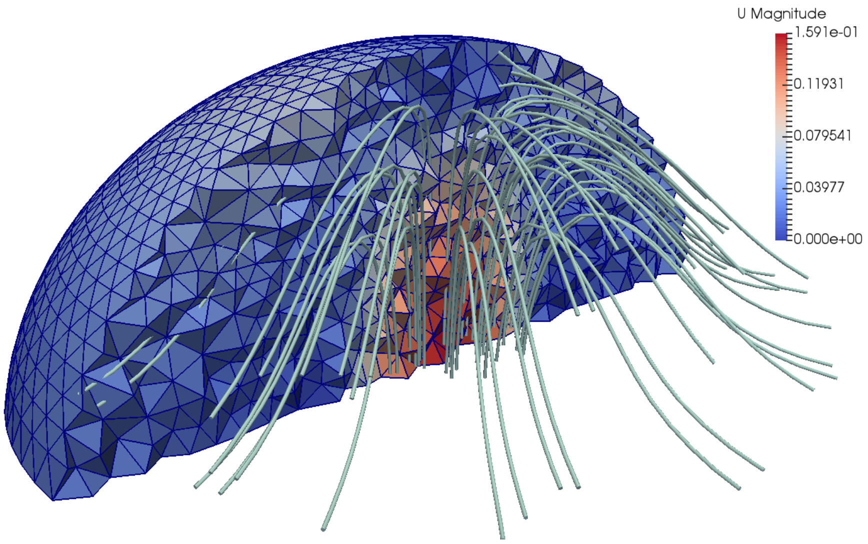

Figure 3: Clipped part of a hemispherical droplet with a radius of $5\,\mathrm{mm}$ for a preliminary study for comparison to experiments. Constant contact angle model with $\theta = 70°$. Inflow of liquid with Poiseuille flow profile and volume flux of $10^{-6}\,\mathrm{m}^3\,\mathrm{s}^{-1}$ through pipe with radius of $2\,\mathrm{mm}$. Mesh color signifies the magnitude of the bulk velocity. The stream lines are indicated with light blue lines.

Relevance

Wetting phenomena are relevant for a wide variety of phenomena in nature and countless technical applications. Especially for technologies where high resolution of the interface is of importance when surfactants come into play the interface tracking method can provide detailed local information. With the implemented contact angle models, it is possible to capture basic wetting phenomena and to evaluate the models performance in comparison to experiments. In addition, the influence of the wall boundary conditions on the flow field can be investigated. The presence of OpenFOAM's finite area method promises an extension and hence a direct comparison to Shikhmurzaev's interface formation model. Furthermore, the incorporation of wetting models into the existing ALE framework will allow to investigate the influence of surfactants on the wetting behavior in the future.

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