Using VOF opensource code for rivulet type flow modeling

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1 Introduction

The flow characteristics of the rivulet type flow are of key importance not only in many areas of chemical engineering but also in numerous other fields of science including even aerospace engineering. Unfortunately, modeling such a flow, one needs to take into account not only the standard set of equation describing liquid flow, but also existence of a free gas-liquid interface and a complex physics occuring on the three phase line of the rivulet. Such complexity results in a very low number of CFD methods available for simulation of the rivulet type flow. Our aim was to the evaluate the possibility of simulating such a flow in the most known and widely used opensource CFD software, OpenFOAM.

The used Cartesian coordinate system as well as the most important symbols are presented in Fig. 1.

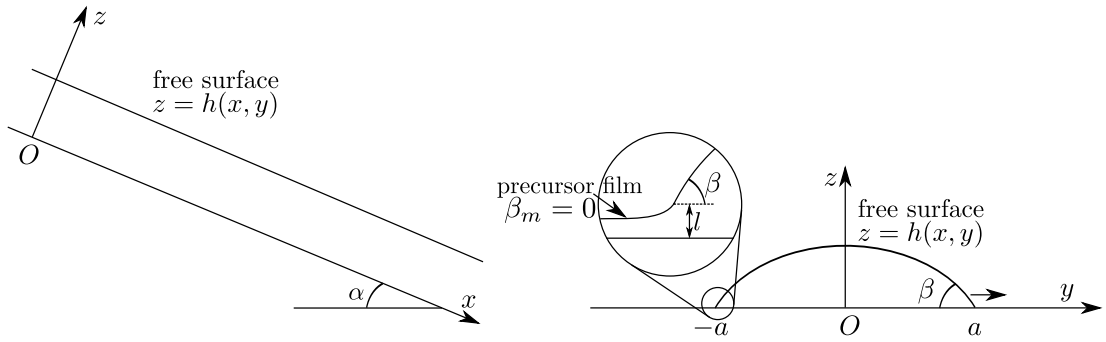

Figure 1: Used coordinate system with the basics of the rivulet spreading notation; α is the plate inclination angle, β and β_m are the apparent and the microscopic contact angles, a is the rivulet half width and l is the problem inner length scale.

Usually, the problems concerning a free interface are modeled through Volume of Fluid (VOF) method, which is implemented in OpenFOAM via interFoam solver. However, OpenFOAM provides also a solver designed for dealing (among other) with film flows, called reactingParcelFilmFoam.

In the presented case, the VOF method for free interface tracking is coupled with Finite Volume Method (FVM) PIMPLE (combination of PISO and SIMPLE) algorithm for solution of velocity and pressure field for both (liquid and gas) phases.

The approach to the physics of the contact (three phase) line of the rivulet depends on the used OpenFOAM solver. Eventhough the interFoam solver provides a possibility of simulation of the evolution of the liquid-solid contact angle based on a physically-realistic model, no corresponding method is available for reactingParcelFilmFoam solver.

In this abstract, we will briefly remind the principle of VOF method, shortly evaluate on different approaches to modeling of force balance on the three phase line and discuss the results obtained using OpenFoam reactingParcelFilmFoam solver.

2 VOF method

The VOF method is an interface tracking technique; however, it tracks fluid volume, hence the interfaces are represented implicitly. The method was first introduced in 1980s by Hirt and Nichols[1] and up to now, it is the most used approach for interface tracking.

The Navier-Stokes equations for an incompressible two phase flow may be written as,

$$u_t + \nabla \cdot (uu) = \frac{1}{\rho} \left(-\nabla p + \nabla \cdot \left(\mu \left(\nabla u + \nabla u^{\mathrm{T}} \right) \right) + F_{st} + F_b \right), \tag{1}$$

where u is the velocity, p pressure, ρ density, F_{st} a volumetric surface tension force and F_b represents any other body forces acting on the fluid. With both fluids considered incompressible, the continuity equation, $\nabla \cdot u = 0$, is valid on the whole domain.

Assuming a two fluid system, a function h is to be defined representing the interface. Function h is set to be equal to 0 in a fluid 1 and 1 in a fluid 2. Also it has to fulfill the advection equation,

$$\partial_t h + u \cdot \nabla h = 0 \tag{2}$$

The volumetric surface tension force may be expressed in the form,

$$F_{st} = \gamma \kappa \delta \vec{n} = \gamma \kappa \nabla h \tag{3}$$

with γ representing the surface tension coefficient, κ curvature, δ the Dirac delta function and $\vec{n}$ the unit normal to the interface.

The fluids density and viscosity are assumed constant in both fluids. However, they may vary between phases and are evaluated using a volume-weighted formulas,

$$\rho = \rho_1 + h \left(\rho_2 - \rho_1 \right), \quad \mu = \mu_1 + h \left(\mu_2 - \mu_1 \right) \tag{4}$$

The principle of VOF method is hidden in its name. The function h, in its discrete form, represents the volume fraction of a cell filled with, in this case, fluid 2. The mesh cells are divided by h to two groups: (i) cells away from the interface, where $h = 0$ or 1 and (ii) cells containing part of the interface, where $h \in (0, 1)$ (see Figure 2).

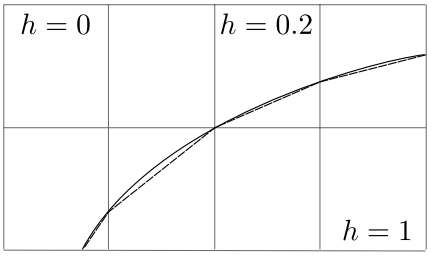

Figure 2: Principle of VOF method. The interface is depicted with a solid line, its geometric reconstruction using piecewise linear function is depicted with a dashed line.

As the equations (1) and (2) are bound together by equation (3), one needs to solve the equation (2) for each cell and time step. Furthermore, equation (2) is usually solved in two steps: (i) a geometric interface reconstrucion, (ii) advection of the reconstructed fluid near interface. An arbitrary function may be used for the interface reconstruction. However, because of the computational complexity of the solution, a piecewise linear function is usually used.

Despite the fact that the method is long and well known, until recently, the VOF simulations of surface tension-driven interfacial phenomena (of which the gravity driven spreading of a rivulet is an example) did suffer from the so-called 'spurious currents'[2], flow induced solely by the discretization and by the lack of convergence with mesh refinement. Moreover, up to our best knowledge, no study was yet published on the theme of presence of spurious currents in OpenFOAM simulations[3].

3 Modeling three phase lines

When calculating the flow dynamics of the problem with moving contact lines, one cannot use the set of standard boundary conditions. The reason is that the no-slip boundary condition causes the surface energy functional to diverge on the contact line[4]. However, this influences only very small part of the problem solution. Furthermore, the scales of the outer and inner solution are usually well separated by an inner length scale, l.

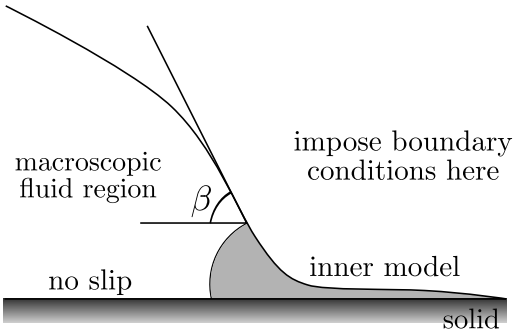

Figure 3: Schematic of procedure for continuum modeling

This leads to a proposition of a general calculation method consisting of finding a microscopic scale solution and of using it as an effective boundary condition for the macroscopic one (see Figure 3).

For the simplest case of a small droplet and a substantial number of simplifying assumptions, a solution of this problem may be obtained analytically[4]. However, the same principle applies also to purely numerical CFD models. The only difference between an analytical and a numerical solution is that in the later case, the inner length scale, l, is not given by the microscopic properties of the problem, but by the resolution of a computational grid.

The connection between the microscopic and macroscopic regions is made through the dynamic contact angle, β.

The studied solvers, interFoam and reactingParcelFilmFoam use different approaches for the β estimation. The interFoam solver uses the so called 'Kistler model'[5], which calculates the dynamic contact angle using the 'Hoffman function', f_H, as follows,

$$\beta = f_H\left(Ca + f_H^{-1}(\beta_{eq})\right), \tag{5}$$

where β_{eq} is the equilibrium contact angle and $Ca = u_{cl}\mu/\gamma$ is the problem Capillary number, in which u_{cl} is the spreading velocity of the contact line. The reactingParcelFilmFoam solver provides no such pre-implemented functionality and the contact angle is simulated through a random number generator with prescribed probability distribution, value range and variance.

4 Results and conclusion

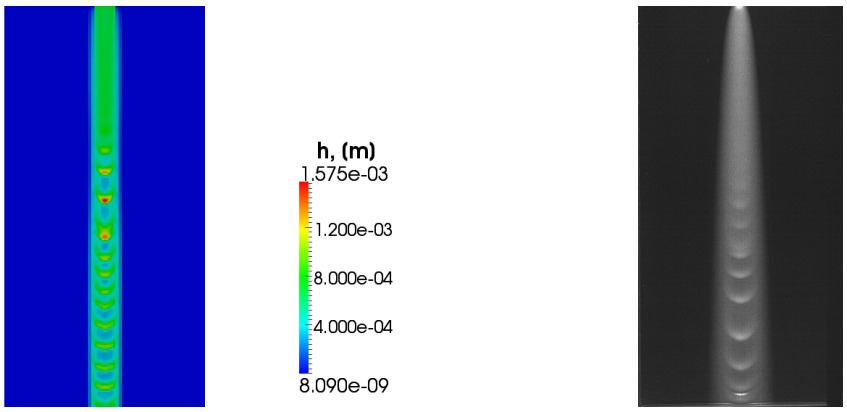

Figure 4: Results of simulation of the rivulet type flow using REACTINGPARCELFILMFOAM. The simulated liquid is DC10 silicon oil of $\gamma = 12\,\mathrm{mN\,m^{-1}}$ and $\mu = 10\,\mathrm{mPa\,s}$. Liquid flow rate is equal to $1.2\,\mathrm{ml\,s^{-1}}$ and plate inclination angle, α, to $\pi/4$. A photo of a rivulet type flow under the same conditions is depicted for reference.

The Figure 4 contains the results of a simulation of one of the simplest cases of rivulet spreading, spreading of a perfectly wetting liquid on a pre-wetted plate. The used solver was REACTINGPARCELFILMFOAM and from the images, it seems that replacing the modeling of the three phase line by a random number generator, while giving seemingly qualitatively accurate results for modeling of unwetting flows, might be a too simplistic approach to the problematics.

In the case of the INTERFOAM solver, while it contains a physically realistic description of the three phase lines, the solver itself seems to be unstable while combining the boundary conditions of the dynamic contact angle and of liquid inflow and outflow.

Eventhough OpenFOAM includes all the needed solvers for successful simulation of rivulet spreading, it did not yet reached the state of providing such capability without a need of the code modifications and/or complex combination of the available solvers. Currently, we are aiming on constructing an OpenFOAM case well suited for the rivulet flow simulations and on testing the code against the available experimental data.

5 References

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