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Using VOF opensource code for rivulet type flow modeling

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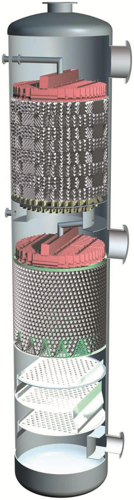
Why to study rivulets

Numerous applications in mass transfer and reaction engineering



[Sulzer ChemTech]

Hydrodynamics

- Fuel cells
  - water management inside PEMFC fuel cells
- Aerospace engineering
  - in flight formation of rivulets on plane wings

Gas-liquid interface

- Packed columns
  - wetting performance
  - mass transfer coefficients
- Catalytic reactors
  - wetting of the catalyst

Why to start with CFD

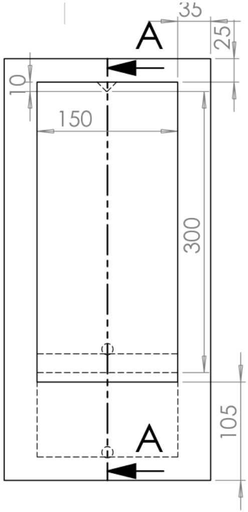
Verification of derived simplified models for spreading rivulet simulation

Derived simplified models

- Gas-liquid interface size calculation
- Velocity field approximation
- Liquid flow rate evolution

Available experimental data

- Gas-liquid interface size measurements using LIF method
- No data for velocity field



Exp. set up CAD

Talk outline

Two parallel approaches to CFD simulations using OPENFOAM

Original geometry and INTERFOAM (IF) solver

- Geometry created using CADs of the experimental set up .
- 3D problem for simulation.
- Used solver based on FVM and VOF.

Simplified geometry and REACTINGPARCELFILMFOAM (RPFF) solver

- Geometry simplified for the problem to be reducible to 2D .
- Used solver specialized for film type flows.

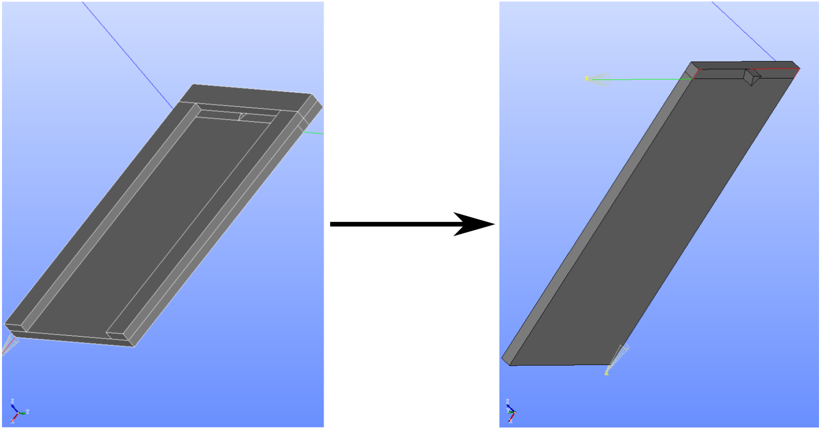
Outline (both cases presented at the same time)

Geometry and Meshing ⇝ BC and Algorithms ⇝ Results

Geometry and Meshing

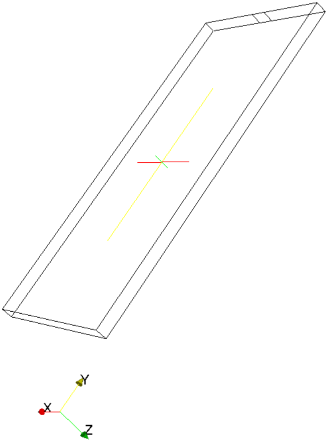
Geometry based on experimental set up

Experimental set up was converted to 3D, computation domain is a negative of it



Simplified geometry

Geometry and direction of liquid inlet was changed to enable problem reduction to 2D



Changes

- Up-most 10 mm including liquid inlet ommitted.
- Triangular liquid inlet perpendicular to the plate $\rightarrow$ rectangular liquid inlet parallel to the plate.

Outcome

- Geometry suitable for use with RPFF solver.

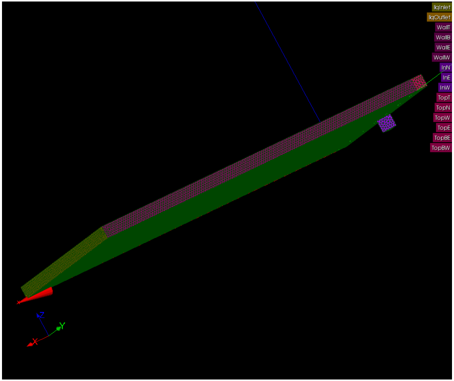
Meshing

Tetragonal 3D mesh and scaled rectangular 2D

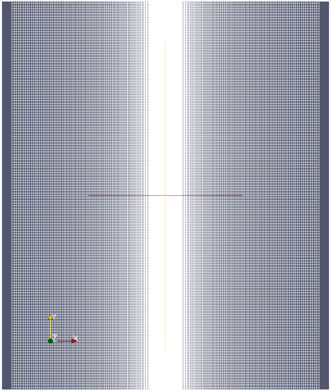
Property	iF	rpfF
Length	310 mm	300 mm
Width	150 mm	150 mm
Height	10 mm	–
Element type	tetrahedrons	rectangles
# of elements	162 709	86 400
Algorithm	NetGen1D2D3D	blockMesh
Software	Salome	OpenFOAM

Meshing

Tetragonal 3D mesh and scaled rectangular 2D mesh



IF mesh

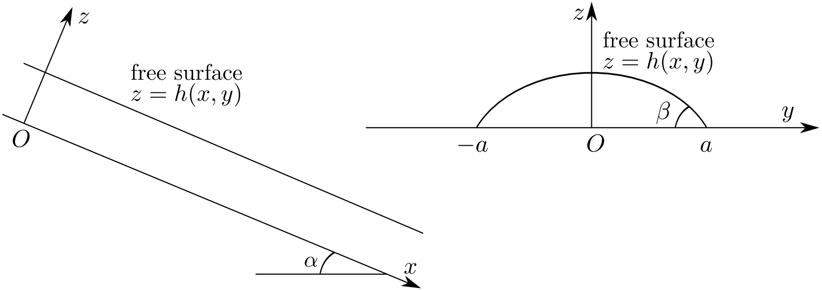


RPFF mesh

Algorithms and BC

Used coordinate system

Cartesian coordinate system and basic notations



Notations

a[m] ......half-width of the rivulet
h[m] .. interface position function
x, y, z[m] ..... coordinate system
$\alpha[-]$ ...... plate inclination angle
$\beta[-]$ ......dynamic contact angle

Solved equations

Isothermal case, incompressible newtonian fluids, flow driven by gravity

Momentum and continuity equations

$$\begin{aligned} u_t + \nabla \cdot (uu) &= \frac{1}{\rho}\left(-\nabla p + \nabla \cdot \left(\mu\left(\nabla u + \nabla u^{\mathrm{T}}\right)\right) + F_{st} + F_b\right) \\ \nabla \cdot u &= 0 \end{aligned}$$

Advection equation for gas-liquid interface (GLI)

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

Notations

$u[\mathrm{m\,s^{-1}}]$	...velocity	F_{st} [N]	..surface tension force
$\mu[\mathrm{Pa\,s}]$	...dynamic viscosity	F_b [N]	..all acting body forces
$\rho[\mathrm{kg\,m^{-3}}]$	...density	$\tilde{h}[-]$	.....GLI tracking function

interFOAM

Description of the solver

Solver description (from the source code)

Solver for 2 incompressible, isothermal immiscible fluids using a VOF (volume of fluid) phase-fraction based interface capturing approach.

Solver set up

Algorithm	FVM (PIMPLE) + VOF
Solver u	Gauss-Seidel
Solver $p_{\rho gh}$	GAMG
Solver p_{corr}	PCG (GAMG)
Solver $\tilde{h}$	smoothSolver (symGaussSeidel)

reactingParcelFilmFOAM

Description of the solver

Solver description (from the source code)

Transient PIMPLE solver for compressible, laminar or turbulent flow with reacting Lagrangian parcels, and surface film modeling.

Solver set up

Algorithm	FVM (PIMPLE)
Solver u	smoothSolver (symGaussSeidel)
Solver $p_{\rho gh}$	smoothSolver (symGaussSeidel)
Solver h	smoothSolver (symGaussSeidel)

Finite Volume Method

Transport equation has to be satisfied in the integral form over V_P around P

Standard form of transport equation for scalar property ϕ

$$\frac{\partial \rho\phi}{\partial t} + \nabla \cdot (\rho u \phi) - \nabla \cdot (\rho \Gamma_\phi \phi) = S_\phi(\phi)$$

Integral form of transport equation for ϕ

$$\int_t^{t+\Delta t} \left[\frac{\partial}{\partial t} \int_{V_P} \rho\phi \,\mathrm{d}V + \int_{V_P} \nabla \cdot (\rho u \phi) \,\mathrm{d}V - \int_{V_P} \nabla \cdot (\rho \Gamma_\phi \phi) \,\mathrm{d}V \right] \mathrm{d}t = \int_{V_P} S_\phi(\phi) \,\mathrm{d}V$$

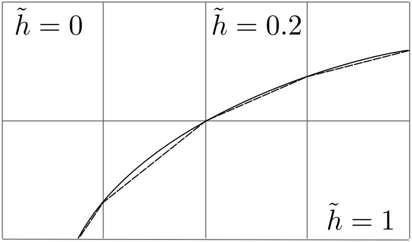
P . centroid of the control volume V_P . . . . . control volume around P

Centroid position:

$$V_P x_P = \int_{V_P} x \,\mathrm{d}V \rightsquigarrow 0 = \int_{V_P} (x - x_p) \,\mathrm{d}V$$

VOF method

Using Volume of fluid method to track the rivulet gas-liquid interface[1, 2]



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

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

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

$$\begin{aligned} F_{st} &= \gamma \kappa \delta \vec{n} = \gamma \kappa \nabla \tilde{h} \\ F_b &= \left(\rho g \sin \alpha, 0, \rho g \cos \alpha \right)^{\mathrm{T}} \end{aligned}$$

PIMPLE algorithm

Combination of SIMPLE and PISO algorithms

SIMPLE - Semi-Implicit Method for Pressure-Linked Equations

1. Guess pressure field, p^*
2. Solve discretized momentum equations and get u^*
3. Calculate pressure and velocity corrections p', u'
4. $p^* = p^* + \alpha p'$, under-relaxation, $\alpha < 1$
5. Repeat 2 – 4 until convergence

PISO - Pressure Implicit with Splitting of Operators

- SIMPLE extended by further corrector step p, u

PIMPLE

- Continuity equation is solved outside of PISO loop
- Velocity field is found in SIMPLE mode
- Pressure field is found in PISO mode

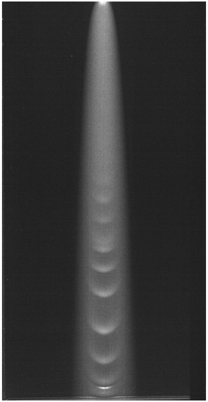
Used boundary conditions

Quantity	Boundary	IF	RPFF
$u [\mathrm{m\,s^{-1}}]$	plate	$u + \lambda \nabla u = 0$	$u + \lambda \nabla u = 0$
	liquid inlet	$u = const.$	$u = const.$
	liquid outlet	$\nabla u = 0$	$\nabla u = 0$
	other	$u = 0$	$u = 0$
$p_{\rho g h}, [-]$	liquid outlet	$p_{\rho g h} = const.$	$p_{\rho g h} = const.$
	other	calculated	calculated
$\tilde{h} [-]$	liquid inlet	$\tilde{h} = 1$	–
	plate	$\beta = f_H \left(Ca + f_H^{-1} (\beta_{eq}) \right)$	–
		$Ca = u_{cl} \mu / \gamma$	–
	other	$\nabla \tilde{h} = 0$	–
	other	calculated	–
$h [\mathrm{m}]$	liquid inlet	–	$h = const.$
	other	–	$\nabla h = 0$

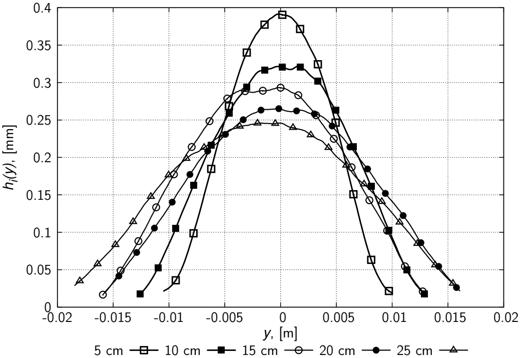
Results

Experimental results

Silicon oil, $\mu \doteq 10^{-2}\,\mathrm{Pa\,s}$, $\gamma \doteq 10^{-2}\,\mathrm{N\,m^{-1}}$ $\rho \doteq 10^{3}\,\mathrm{kg\,m^{-3}}$, $\alpha = \pi/4$, $Q = 2.4\,\mathrm{ml\,s^{-1}}$



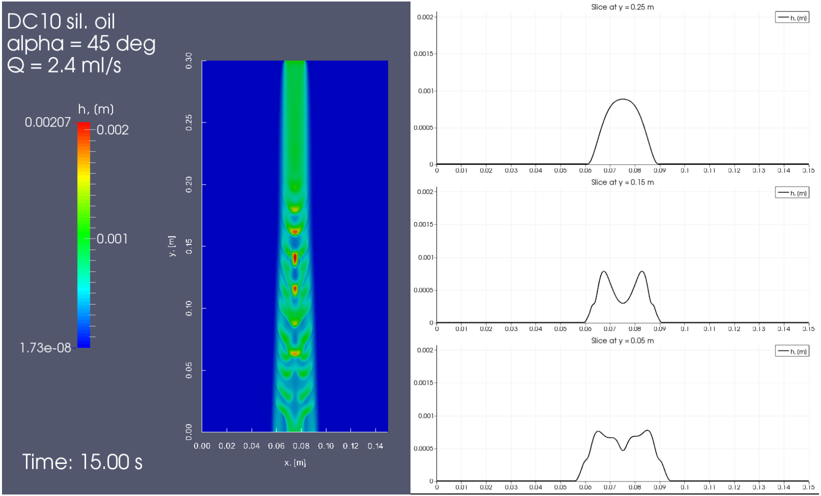
rivulet photo



interface shape along the rivulet

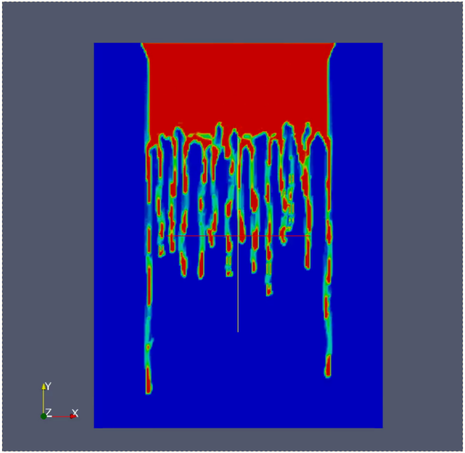
reactingParcelFilmFOAM

Silicon oil, $\mu \doteq 10^{-2}\,\mathrm{Pa\,s}$, $\gamma \doteq 10^{-2}\,\mathrm{N\,m^{-1}}$ $\rho \doteq 10^{3}\,\mathrm{kg\,m^{-3}}$, $\alpha = \pi/4$, $Q = 2.4\,\mathrm{ml\,s^{-1}}$



reactingParcelFilmFOAM

Detail of rivulet without underlying wetting film and random contact angle



Conclusions and Outlook

Conclusions and Outlook

No method for accurate spreading rivulet modeling is implemented in OPENFOAM

interFoam solver

- Uses physically correct implementation of force balance at the three phase line
- Unrealistic demands on mesh refinement

reactingParcelFilmFoam solver

- Suitable for thin film modeling
- Contact line movement is modeled based on random contact angle
- Gives reasonable and physically defensible results only for spreading on wetted plate (no three phase line force balance is needed)

Outlook

Provide suitable implementation for modeling of a rivulet spreading on non-wetted plate

Implement interFoam contact angle modeling in reactingParcelFilmFOAM

- Implement contact angle modeling based on Kistler model[5] in reactingParcelFilmFoam solver

$$\beta = f_H \left(Ca + f_H^{-1}(\beta_{eq}) \right) , \quad Ca = u_{cl} \frac{\mu}{\gamma},$$

  where f_H is Hoffman function

- Such an implementation is available for interFoam solver and may be reused for reactingParcelFilmFoam

References

In order of appearance

[1] W. Hirt, B. D. Nichols: *Volume of Fluid (VOF) method for the dynamics of free boundaries*, In: J. Comp. Phys., 1981, *39* pp. 201 – 225.

[2] S. Afkhami, M. Bussmann: *Height functions for applying contact angles to 3D VOF simulations*, In: Int. J. Num. Meth. in Fluids, 2008.

[3] S. S. Deshpande, L. Anumolu, M. F. Trujillo: *Evaluating the performace of the two-phase flow solver interFoam*, In: Comp. Sc. & Disc., 2012, *5*.

[4] D. Bonn, J. Eggers, J. Indekeu, J. Meunier, E. Rolley: *Wetting and Spreading*, In: Rev. Mod. Phys., 2009, *81*, pp. 739–805.

[5] S. Sikalo, H.-D. Wilhelm, I. V. Roisman, S. Jakirlic, C. Tropea: *Dynamic contact angle of spreading droplets: Experiments and simulations*, In: Phys. of Fluids, 2005, *17*.

Acknowledgments

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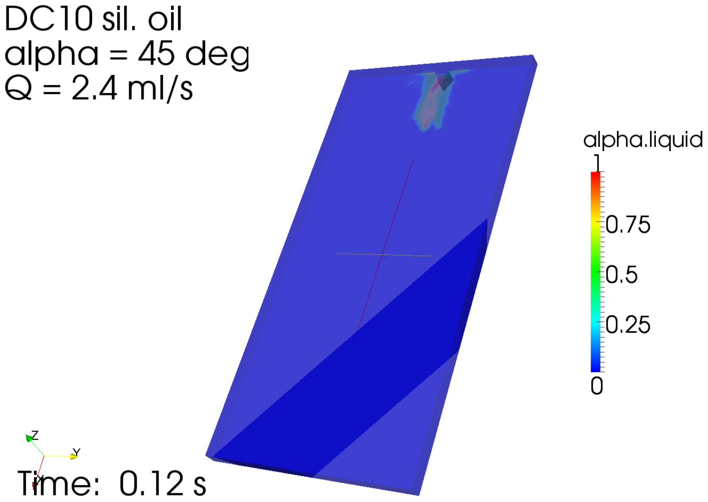
Thank you for your attention

interFOAM – Numerically unstable

Silicon oil, $\mu \doteq 10^{-2}\,\mathrm{Pa\,s}$, $\gamma \doteq 10^{-2}\,\mathrm{N\,m^{-1}}$ $\rho \doteq 10^{3}\,\mathrm{kg\,m^{-3}}$, $\alpha = \pi/4$, $Q = 2.4\,\mathrm{ml\,s^{-1}}$

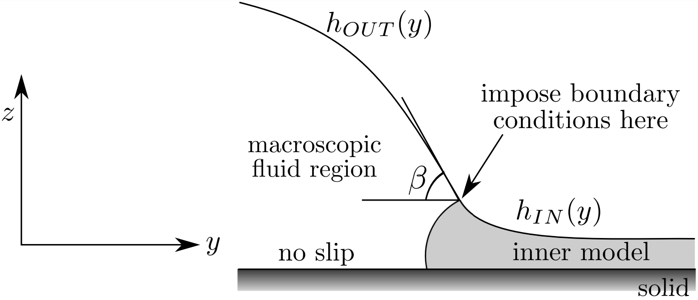


Modeling three phase lines

A very fine mesh is needed in contact line region

Thin film governing equation - outer and inner

$$h_t + \frac{\gamma}{3\mu}\frac{\partial}{\partial a}\left(h^3 h_{aaa}\right) = 0, \qquad h_t + \frac{1}{3\mu}\frac{\partial}{\partial a}\left[\left(h^3 + 3\lambda h^2\right)\gamma h_{aaa}\right] = 0$$



Consequence

For being able to accurately predict the movement of three phase line a very fine mesh is needed in contact line region