Using VOF opensource code for rivulet type flow modeling

Martin Isoz

UCT Prague

19.– 23. 1. 2015
Why to study rivulets
Numerous applications in mass transfer and reaction engineering

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

[Sulzer ChemTech]

Martin Isoz – UCT Prague
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

Martin Isoz – UCT Prague
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 REACTING PARCEL FILM FOAM (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

Martin Isoz – UCT Prague
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 → rectangular liquid inlet parallel to the plate.

Outcome

- Geometry suitable for use with RPF F solver.
# Meshing

Tetragonal 3D mesh and scaled rectangular 2D

<table>
<thead>
<tr>
<th>Property</th>
<th>IF</th>
<th>RPFF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length</td>
<td>310 mm</td>
<td>300 mm</td>
</tr>
<tr>
<td>Width</td>
<td>150 mm</td>
<td>150 mm</td>
</tr>
<tr>
<td>Height</td>
<td>10 mm</td>
<td>–</td>
</tr>
<tr>
<td>Element type</td>
<td>tetrahedrons</td>
<td>rectangles</td>
</tr>
<tr>
<td># of elements</td>
<td>162 709</td>
<td>86 400</td>
</tr>
<tr>
<td>Algorithm</td>
<td>NETGEN1D2D3D</td>
<td>BLOCKMESH</td>
</tr>
<tr>
<td>Software</td>
<td>SALOME</td>
<td>OPENFOAM</td>
</tr>
</tbody>
</table>

Martin Isoz – UCT Prague
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

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

\( z = h(x, y) \) — free surface
Solved equations
Isothermal case, incompressible newtonian fluids, flow driven by gravity

Momentum and continuity equations

\[
\begin{align*}
\frac{D}{Dt} \mathbf{u} + \nabla \cdot (\mathbf{uu}) &= \frac{1}{\rho} \left( -\nabla p + \nabla \cdot (\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) + \mathbf{F}_{st} + \mathbf{F}_b \right) \\
\nabla \cdot \mathbf{u} &= 0
\end{align*}
\]

Advection equation for gas-liquid interface (GLI)

\[
\partial_t \tilde{h} + \mathbf{u} \cdot \nabla \tilde{h} = 0
\]

Notations

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Unit</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(u)</td>
<td>(\text{m s}^{-1})</td>
<td>velocity</td>
</tr>
<tr>
<td>(\mu)</td>
<td>(\text{Pa s})</td>
<td>dynamic viscosity</td>
</tr>
<tr>
<td>(\rho)</td>
<td>(\text{kg m}^{-3})</td>
<td>density</td>
</tr>
<tr>
<td>(\mathbf{F}_{st})</td>
<td>(\text{N})</td>
<td>surface tension force</td>
</tr>
<tr>
<td>(\mathbf{F}_b)</td>
<td>(\text{N})</td>
<td>all acting body forces</td>
</tr>
<tr>
<td>(\tilde{h})</td>
<td>((-)</td>
<td>GLI tracking function</td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Solver</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u$</td>
<td>$p_{\rho gh}$</td>
</tr>
<tr>
<td>FVM (PIMPLE) + VOF</td>
<td>Gauss-Seidel</td>
</tr>
</tbody>
</table>

Martin Isoz – UCT Prague
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

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>FVM (PIMPLE)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solver $u$</td>
<td>smoothSolver (symGaussSeidel)</td>
</tr>
<tr>
<td>Solver $p_{\rho gh}$</td>
<td>smoothSolver (symGaussSeidel)</td>
</tr>
<tr>
<td>Solver $h$</td>
<td>smoothSolver (symGaussSeidel)</td>
</tr>
</tbody>
</table>
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 $\phi$**

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

**Integral form of transport equation for $\phi$**

$$\int_t^{t+\Delta t} \left[ \frac{\partial}{\partial t} \int_{V_P} \rho \phi \, dV + \int_{V_P} \nabla \cdot (\rho u \phi) \, dV - \int_{V_P} \nabla \cdot (\rho \Gamma \phi \phi) \, dV \right] \, dt$$

$$= \int_{V_P} S_\phi(\phi) \, dV$$

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

Centroid position:

$$V_P x_P = \int_{V_P} x \, dV \sim 0 = \int_{V_P} (x - x_P) \, dV$$

Martin Isoz – UCT Prague
VOF method
Using Volume of fluid method to track the rivulet gas-liquid interface[1, 2]

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

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

\[ \rho = \rho_1 + \tilde{h} (\rho_2 - \rho_1) \]

\[ \mu = \mu_1 + \tilde{h} (\mu_2 - \mu_1) \]

\[ F_{st} = \gamma \kappa \delta \tilde{n} = \gamma \kappa \nabla \tilde{h} \]

\[ F_b = (\rho g \sin \alpha, 0, \rho g \cos \alpha)^T \]
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

Martin Isoz – UCT Prague
### Used boundary conditions

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Boundary</th>
<th>IF</th>
<th>RPFF</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u [\text{m s}^{-1}]$</td>
<td>plate</td>
<td>$u + \lambda \nabla u = 0$</td>
<td>$u + \lambda \nabla u = 0$</td>
</tr>
<tr>
<td></td>
<td>liquid inlet</td>
<td>$u = \text{const.}$</td>
<td>$u = \text{const.}$</td>
</tr>
<tr>
<td></td>
<td>liquid outlet</td>
<td>$\nabla u = 0$</td>
<td>$\nabla u = 0$</td>
</tr>
<tr>
<td></td>
<td>other</td>
<td>$u = 0$</td>
<td>$u = 0$</td>
</tr>
</tbody>
</table>

| $p_{\rho gh}, [-]$ | liquid outlet      | $p_{\rho gh} = \text{const.}$ | $p_{\rho gh} = \text{const.}$ |
|                  | other             | calculated                     | calculated                     |

| $\tilde{h} [-]$ | liquid inlet      | $\tilde{h} = 1$               |                                 |
|                 | plate             | $\beta = f_H (Ca + f_H^{-1}(\beta_{eq}))$ |                                 |
|                 | $Ca = u_{cl} \mu / \gamma$ |                                |                                 |
|                 | other             | $\nabla \tilde{h} = 0$         |                                 |
|                 | other             | calculated                     |                                 |

| $h [\text{m}]$ | liquid inlet      | $h = \text{const.}$            |                                 |
|                | other             | $\nabla h = 0$                 |                                 |
Results
Experimental results
Silicon oil, $\mu = 10^{-2} \text{ Pa s}$, $\gamma = 10^{-2} \text{ N m}^{-1}$ $\rho = 10^3 \text{ kg m}^{-3}$, $\alpha = \pi/4$, $Q = 2.4 \text{ ml s}^{-1}$

rivulet photo

interface shape along the rivulet

Martin Isoz – UCT Prague
**reactingParcelFilmFOAM**

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

**DC10 sil. oil**

alpha = 45 deg

$Q = 2.4$ ml/s

Time: 15.00 s
reactingParcelFilmFOAM
Detail of rivulet without underlying wetting film and random contact angle
Conclusions and Outlook
No method for accurate spreading rivulet modeling is implemented in OpenFOAM

**Conclusions and Outlook**

**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

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

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


Acknowledgments

The presented work was supported by IGA of ICT Prague, under the grant number A2_FCHI_2014_001.
Thank you for your attention
interFOAM – Numerically unstable

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

DC10 sil. oil
alpha = 45 deg
$Q = 2.4$ ml/s
Modeling three phase lines
A very fine mesh is needed in contact line region

Thin film governing equation - outer and inner

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

Consequence

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

Martin Isoz – UCT Prague