Efficient simulation techniques for incompressible two-phase flow

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Motivation

**CFD simulation tool:** *Droplet generation and deposition*

**Simulation results:** *dispersity, droplet sizes, splash thickness/diameter (shape)*

**Simulation parameters:** *physical and geometrical parameters, operation conditions*

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**Regions of interest**

- Dynamics of droplet generation (B7)
  - Turbulence
  - Modulation

- Dynamics of droplet deposition (B1)
  - Solidification
  - Contact angle
  - Interaction
  - Roughness
Methods for B1 and B7

- Mass conservative FEM levelset approach with „exact“ interphase reconstruction. Implicit treatment of the surface tension force term
- Fast solvers (parallel multigrid) for scalar equations and for the Pressure-Poisson equation supporting large density jumps
- Systematic validation and benchmarking (CFX, FEMLAB, FLUENT, OpenFOAM).
- Incorporation of adaptive grid deformation techniques and/or hanging nodes
The incompressible Navier-Stokes with the heat equation:

\[ \rho \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) - \nabla \cdot \left( \mu + \mu_T \right) \left( \nabla \mathbf{v} + (\nabla \mathbf{v})^T \right) \right] + \nabla p = \mathbf{f}_{ST} + \rho \mathbf{g} \]

\[ \rho c_p \left( \frac{\partial \Theta}{\partial t} + \mathbf{v} \cdot \nabla \Theta \right) - \nabla \cdot (k \nabla \Theta) = \rho g(\Theta), \quad \nabla \cdot \mathbf{v} = 0 \]

Interphase tension force:

\[ \mathbf{f}_{ST} = \sigma \kappa \mathbf{n}, \quad \kappa = -\nabla \cdot \mathbf{n} \quad \text{on} \quad \Gamma \]

Dependency of physical quantities:

\[ \mu = \mu(D(\mathbf{v}), \Gamma), \quad \rho = \rho(\Gamma) \]

Interphase indicator

\[ \frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0 \]

with reinitialization

\[ \frac{\partial \phi}{\partial \tau} + \mathbf{n} \cdot \nabla \phi = S(\phi) \]

Turbulence model – standard/modified \( k - \varepsilon \) model:

\[ \frac{\partial k}{\partial t} + \nabla \cdot \left( k \mathbf{u} - \frac{v_T}{\sigma_k} \nabla k \right) = P_k - \varepsilon \]

\[ v_T = C_\mu \frac{k^2}{\varepsilon} \]

\[ \frac{\partial \varepsilon}{\partial t} + \nabla \cdot \left( \varepsilon \mathbf{u} - \frac{v_T}{\sigma_\varepsilon} \nabla \varepsilon \right) = \frac{\varepsilon}{k} \left( C_1 P_k - C_2 \varepsilon \right) \]

\[ P_k = v_T \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right]^2 \]

Only for the gas phase!
Efficient flow solver - **FeatFlow**

**Main features of the FeatFlow approach:**
- Parallelization based on domain decomposition
- High order discretization schemes
- Use of unstructured meshes
- Newton-Multigrid solvers
- FCT & EO stabilization techniques
- Adaptive grid deformation

**Benchmarked applications**
- Laminar Newtonian flows
- Laminar non-Newtonian flows
- Turbulent flows (k-epsilon)
- Fluid-structure interaction
- Immiscible laminar two-phase flow

**Discretization:**
- Navier-Stokes: FEM $Q_2/P_1$ in space
- Level Set: DG-FEM $P_1$ in space
- Crank-Nicholson scheme in time
Efficient interphase capturing method

Level Set Method (➔ “smooth“ distance function)

\[ \frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0 \]

**Benefits:**
- Provides an accurate representation of the interphase
- Provides other auxiliary quantities (normal, curvature)
- Allows topology changes
- Treatment of viscosity, density and surface tension without explicit representation of the interphase
- Adaptive grid advantageous, but not necessary

**Problems:**
- It is not conservative ➔ mass loss
- Needs to be reinitialized to maintain its distance property
- Higher order discretization: possible, but necessary?
Problems and Challenges

- **Steep gradients** of physical quantities at the interphase

- **Reinitialization** (smoothed sign function, artificial movement of the interphase)

- **Mass conservation** (during advection and reinitialization of the Level Set function)

- Representation of **interphacial tension**: CSF, Line Integral, Laplace-Beltrami, Phasefield, etc.

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Cellwise averaging

\[ \rho_e = x \rho_1 + (1-x) \rho_2, \quad \mu_e = x \mu_1 + (1-x) \mu_2 \]

PDE based reinitialization

\[ \frac{\partial \phi}{\partial \tau} + \mathbf{u} \cdot \nabla \phi = S(\phi) \quad \mathbf{u} = S(\phi) \frac{\nabla \phi}{|\nabla \phi|} \quad \iff \quad |\nabla \phi| = 1 \]

CSF smoothening with Dirac \( \delta \) function

\[ f_{ST} = \sigma \kappa \mathbf{n} \delta(x, \varepsilon) \]
Validation for the rising bubble problem

Free parameters to adjust Eo and Mo:

\[ Eo = \frac{g_z \Delta \rho gl d_b^2}{\sigma gl} \]

\[ Mo = \frac{g_z \mu l^4 \Delta \rho gl}{\rho l^2 \sigma gl} \]


Rising bubble – Case B

\[ \rho_1 : \rho_2 = \mu_1 : \mu_2 = 1:100 \]

\[ \text{Eo} = 9.71 \quad \text{Mo} = 0.100 \]

\[ \text{Re}_{\text{Sim}} = 4.60 \quad \text{Re}_{\text{graph}} = 5.60 \]

Rising bubble – Case C

\[ \rho_1 : \rho_2 = \mu_1 : \mu_2 = 1 : 100 \quad E_0 = 97,1 \quad M_0 = 0,971 \]

\[ \text{Re}_{\text{Sim}} = 20,0 \quad \text{Re}_{\text{graph}} = 18,0 \]

Rising bubble – Case D

$\rho_1 : \rho_2 = \mu_1 : \mu_2 = 1:100$

$E_0 = 97.1$  $M_0 = 1000$

$Eo=97,1$  $Mo=1000$


$R_{e_{Sim}} = 1.50$  $R_{e_{graph}} = 2.03$
Benchmarking on experimental results

Continuous phase:

Glucose-Water mixture
\[ \mu_D = 500 \text{mPa} \text{s} \]
\[ \rho_D = 972 \text{kg m}^{-3} \]
\[ \dot{V}_D = 3.64 \text{ml min}^{-1} \]
\[ \sigma_{CD} = 0.034 \text{N m}^{-1} \]

Silicon oil
\[ \mu_C = 500 \text{mPa s} \]
\[ \rho_C = 1340 \text{kg m}^{-3} \]
\[ \dot{V}_C = 99.04 \text{ml min}^{-1} \]

Dispersed phase:

Experimental Set-up with AG Walzel (BCI/Dortmund)

Validation parameters:
- frequency of droplet generation
- droplet size
- stream length
Benchmarking on experimental results

<table>
<thead>
<tr>
<th></th>
<th>Separation frequency [Hz]</th>
<th>Droplet size [dm]</th>
<th>Stream Length [dm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exp</td>
<td>0.58</td>
<td>0.062</td>
<td>0.122</td>
</tr>
<tr>
<td>Sim</td>
<td>0.6</td>
<td>0.058</td>
<td>0.102</td>
</tr>
</tbody>
</table>

Exp. results → Group of Prof. Walzel
BCI/Dortmund
Validation for wide range of experiments

**Experimental results: Group of Prof. Walzel BCI/Dortmund**

**Example 1:**
\( \dot{V}_D = 1.1 \text{ ml/min} \)
\( \dot{V}_C = 13.0 \text{ ml/min} \)
\( \dot{V}_D/\dot{V}_{tot} = 0.08 \)

**Example 2:**
\( \dot{V}_D = 1.5 \text{ ml/min} \)
\( \dot{V}_C = 41.1 \text{ ml/min} \)
\( \dot{V}_D/\dot{V}_{tot} = 0.04 \)

**Example 3:**
\( \dot{V}_D = 2.5 \text{ ml/min} \)
\( \dot{V}_C = 123.2 \text{ ml/min} \)
\( \dot{V}_D/\dot{V}_{tot} = 0.02 \)

**Effects of contact angle?**
Influence of modulation

No Regulation
Flowrate: 100%
Capillary: STD
Droplet size: 5.2mm

Regulated
Flowrate: 100%
Capillary: STD
Droplet size: 5.0mm

Regulated
Flowrate: 150%
Capillary: STD
Droplet size: 5.7mm

Regulated
Flowrate: 75%
Capillary: 50% STD
Droplet size: 4.5mm

Resulting operation envelope:
- Size: 4.5 mm – 5.7 mm
- Volume: 0.38 cm³ – 0.77 cm³
Droplet deposition


+ Contact angle & interaction & solidification!
Solidification

\[ \rho c_p \left( \frac{\partial \Theta}{\partial t} + \mathbf{v} \cdot \nabla \Theta \right) - \nabla \cdot (k \nabla \Theta) = \rho g(\Theta) \]

\[ f \]

\[ H_L(\Theta) = \begin{cases} 
L, & \Theta > \Theta_L \\
\frac{\Theta - \Theta_s}{\Theta_L - \Theta_s}, & \Theta_s \leq \Theta < \Theta_L \\
0, & \Theta < \Theta_s 
\end{cases} \]

- Enthalpy method for binary alloy solidification
- The condition of zero velocity in solid regions is accounted with:
  - Temperature dependent viscosity
  - Fictitious boundary method (FBM)

Influence on impinging droplets

Without solidification

With solidification

Validation of turbulence models

- Standard $k$-$\varepsilon$ model
- Chien’s low Re $k$-$\varepsilon$ model

+ Boundary conditions!

Channel flow for $Re_\tau = \frac{du_\tau}{\nu} = 395$

$y^+ = \frac{u_\tau y}{\nu}$, $u^+ = \frac{u_x}{u_\tau}$, $k^+ = \frac{k}{u_\tau^2}$, $\varepsilon^+ = \frac{\varepsilon \nu}{u_\tau^4}$

Backward facing step for $Re_\tau = \frac{HU}{\nu} = 47,625$

Reattachment length $5.0 < x_{r,\text{literature}} < 6.5$
Conclusions and future plans

Overview of the modules of the desired simulation tool

<table>
<thead>
<tr>
<th>module:</th>
<th>status:</th>
</tr>
</thead>
<tbody>
<tr>
<td>CFD solver</td>
<td>Parallelized, multi-grid based, high order, Benchmarkarded</td>
</tr>
<tr>
<td>Level Set</td>
<td>Parallelized and equipped with reinitialization, Benchmarkarked</td>
</tr>
<tr>
<td>Heat equation</td>
<td>Parallelized, Solidification is tested and verified in 2D</td>
</tr>
<tr>
<td>Turbulence model</td>
<td>Sequential, tested and verified in 3D, low/high Reynolds number extensions</td>
</tr>
</tbody>
</table>

Dynamics of droplet deposition

- CFD solver
- Level Set
- Heat equation
- Solidification

Dynamics of droplet generation

- CFD solver
- Level Set
- Turbulence model
- Modulation

Experimental/computational reference results ⇒ Proposal of benchmark problems