3D-Surface Engineering für Werkzeug-systeme der Blechformteilefertigung

- Erzeugung, Modellierung, Bearbeitung -

Efficient simulation techniques for incompressible two-phase flow

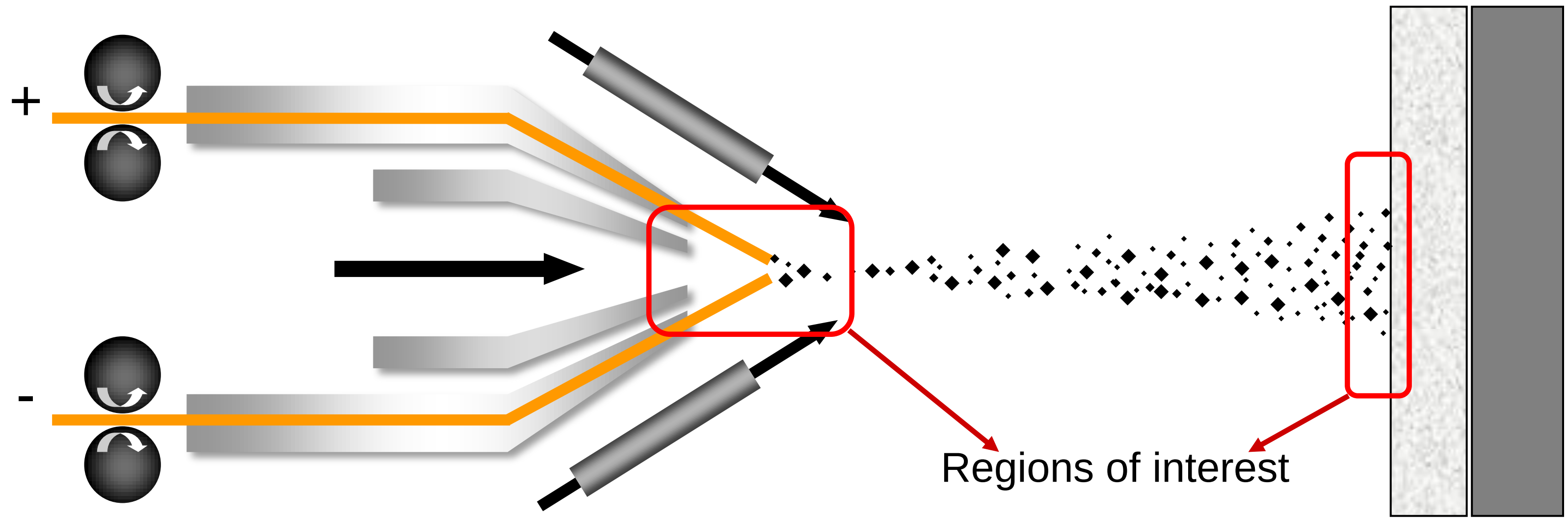
O. Mierka, O. Ouazzi, T. Theis, S. Turek

TP B7

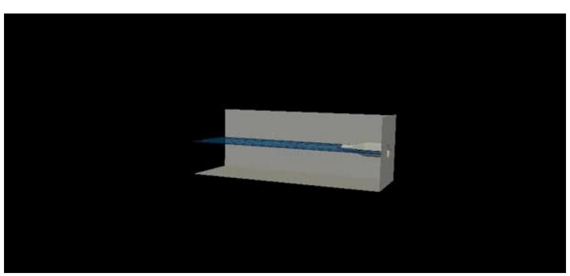
4. öffentliches Kolloquium
15. November 2011

Motivation

CFD simulation tool: *<u>Droplet generation and deposition</u>*
Simulation results: *dispersity, droplet sizes, splash thickness/diameter (shape)*
Simulation parameters: *physical and geometrical parameters, operation conditions*

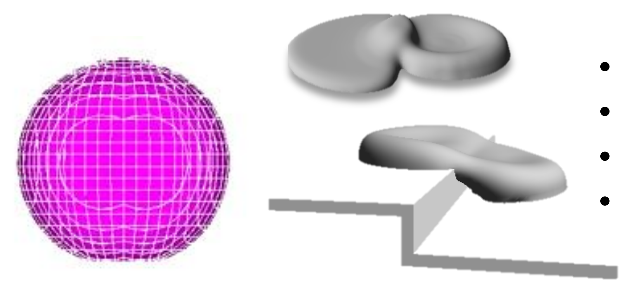


Dynamics of droplet generation (B7)



- Turbulence
- Modulation

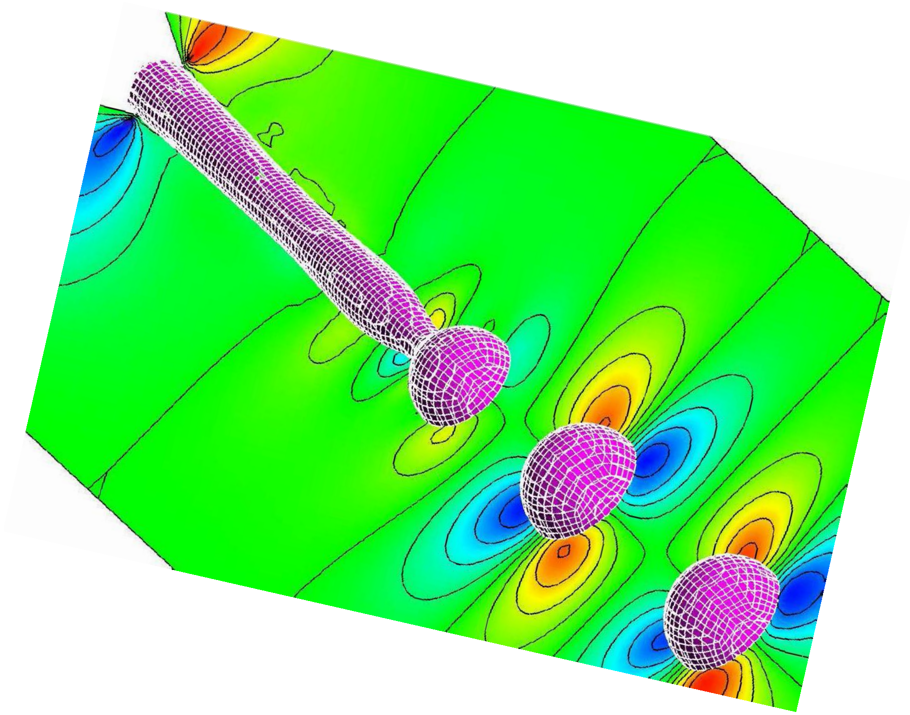
Dynamics of droplet deposition (B1)

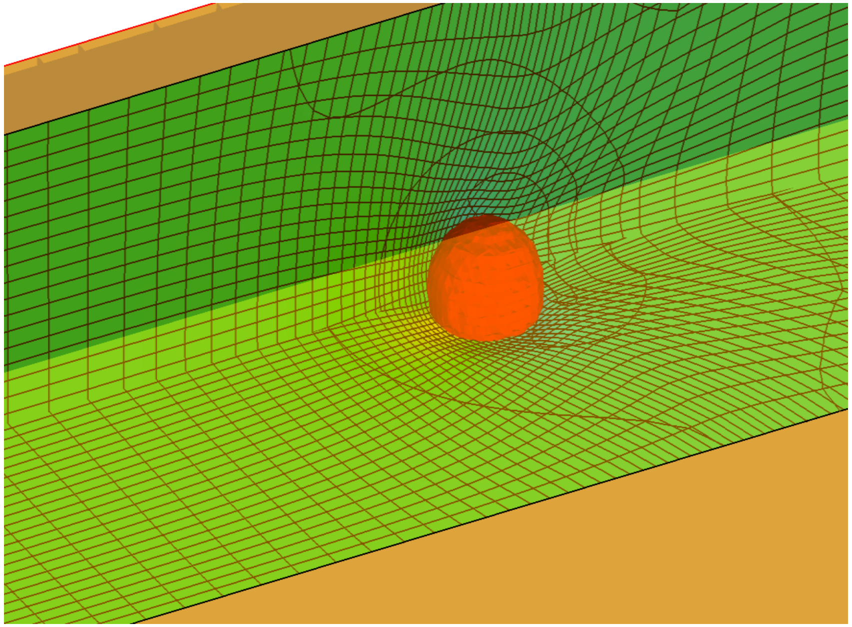


- Solidification
- Contact angle
- Interaction
- Roughness

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





Governing equations

The incompressible Navier Stokes with the heat equation

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

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

turbulent effects

Interphase tension force

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

unknown interphase location

Dependency of physical quantities

$$\mu=\mu\left(D\left(\mathbf{v}\right),\Gamma\right),\quad \rho=\rho\left(\Gamma\right)$$

+

Interphase indicator

Level Set

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

with reinitialization

$$\frac{\partial\phi}{\partial\tau}+\mathbf{n}\cdot\nabla\phi=S\left(\phi\right)$$

+

Turbulence model – standard/modified $k-\varepsilon$ model

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

$$\frac{\partial \varepsilon}{\partial t}+\nabla\cdot\left(\varepsilon\mathbf{u}-\frac{\nu_T}{\sigma_\varepsilon}\nabla \varepsilon\right)=\frac{\varepsilon}{k}\left(C_1P_k-C_2\varepsilon\right)$$

$$\nu_T=C_\mu\frac{k^2}{\varepsilon}$$

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

Only for the gas phase!

Efficient flow solver - FeatFlow

Main features of the FeatFlow approach:

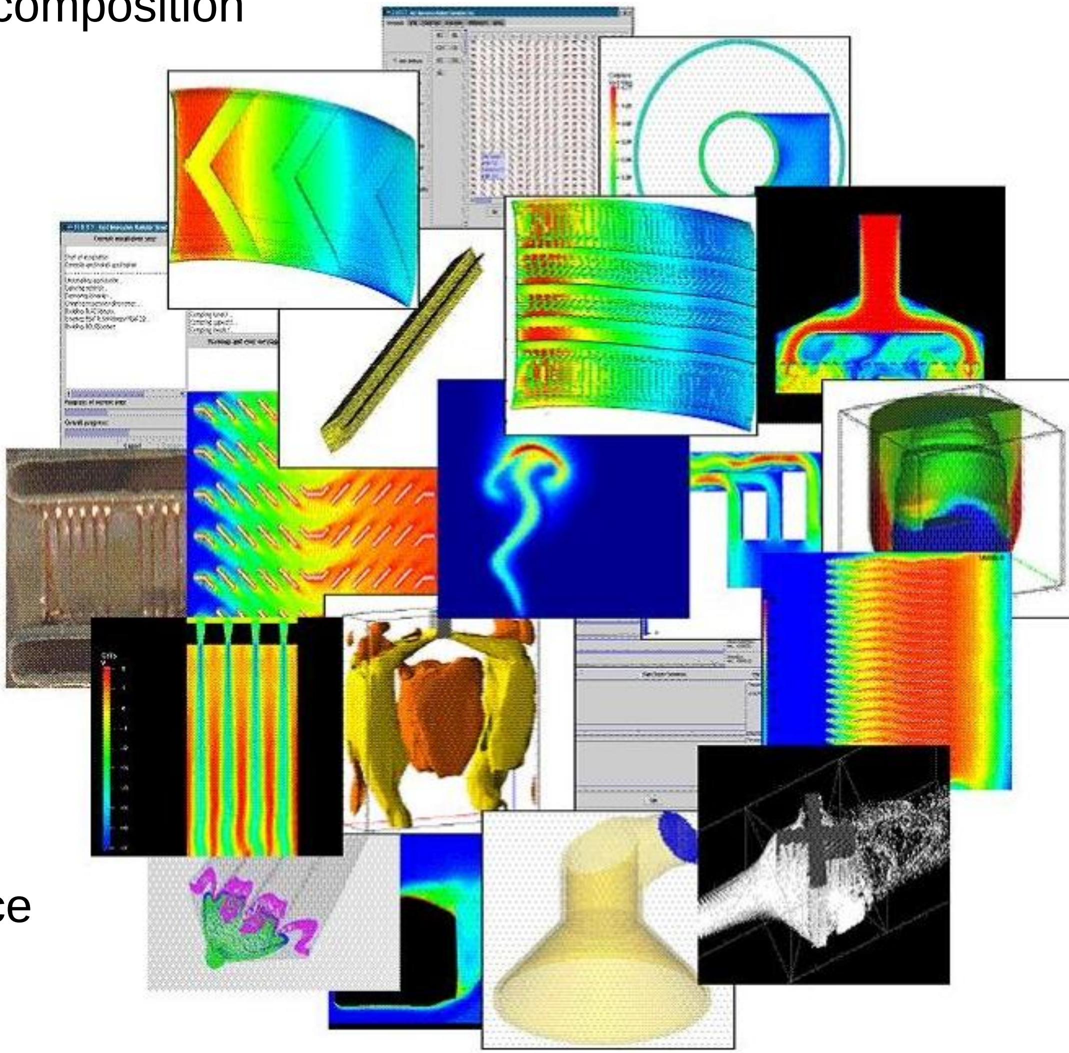
- Parallelization based on domain decomposition
- High order discretization schemes
- Use of unstructured meshes
- Newton-Multigrid solvers
- FCT & EO stabilization techniques
- Adaptive grid deformation

Benchmarked applications

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

Discretization:

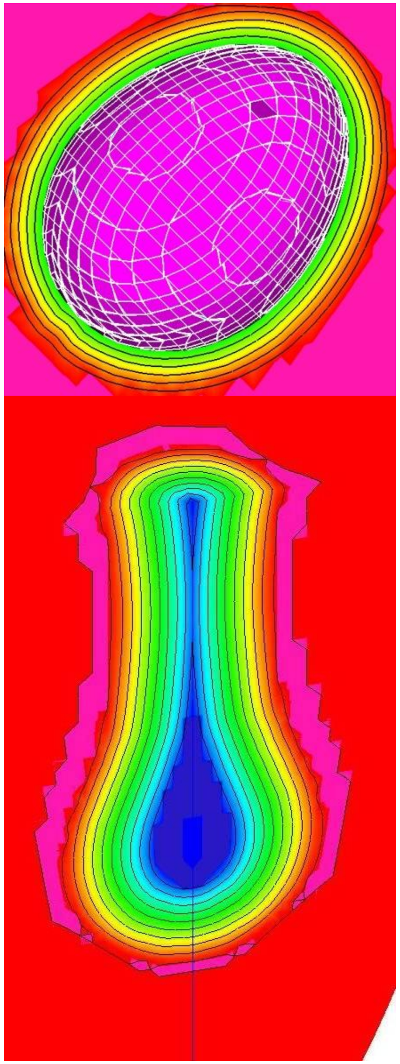
- Navier-Stokes: FEM Q_2/P_1 in space
- Level Set: DG-FEM P_1 in space
- Crank-Nicholson scheme in time



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

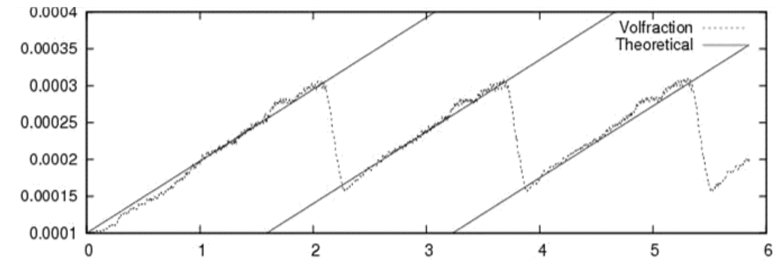
- **Steep gradients** of physical quantities at the interphase
- **Reinitialization** (smoothed sign function, artificial movement of the interphase)
- **Mass conservation** (during advection and reinitialization of the Level Set function)
- Representation of **interphacial tension**: CSF, Line Integral, Laplace-Beltrami, Phasefield, *etc.*

Cellwise averaging

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

PDE based reinitialization

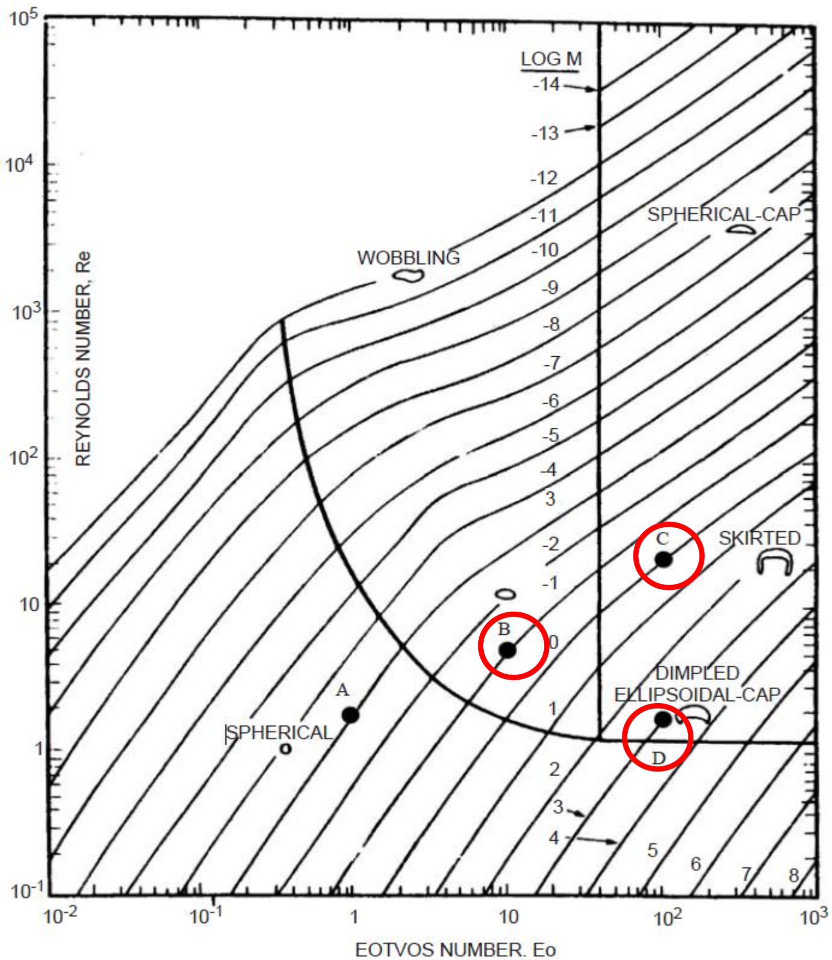
$$\frac{\partial \phi}{\partial \tau} + \mathbf{u}\cdot\nabla\phi = S(\phi) \qquad \mathbf{u} = S(\phi)\frac{\nabla\phi}{|\nabla\phi|} \quad \Leftrightarrow \quad |\nabla\phi| = 1$$

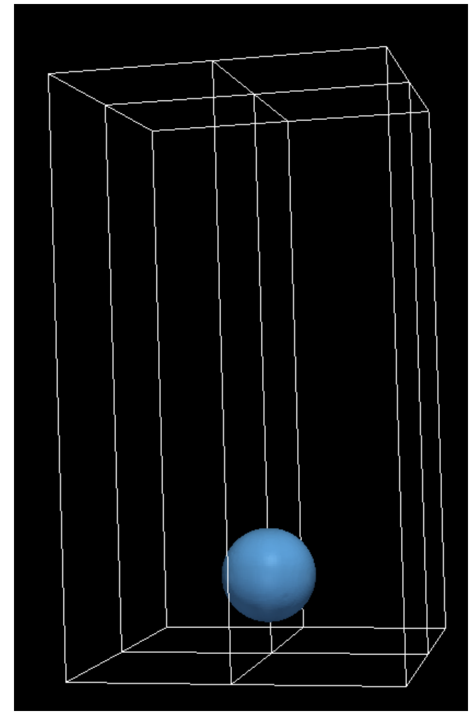


CSF smoothening with Dirac δ function

$$\mathbf{f}_{\mathrm{ST}} = \sigma\kappa\mathbf{n}\delta(x,\varepsilon)$$

Validation for the rising bubble problem





Free parameters to adjust Eo and Mo: $g_z \quad \sigma_{gl}$

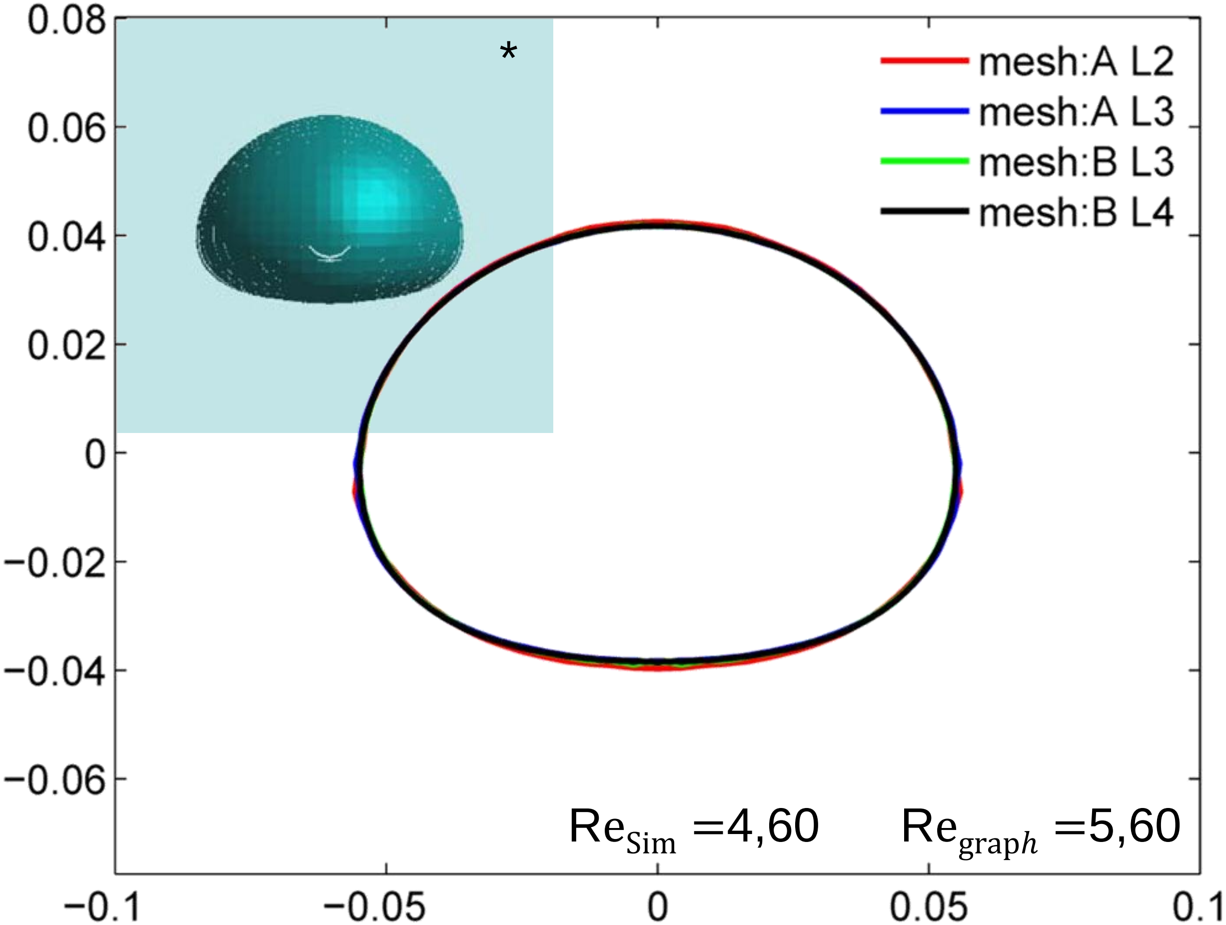
$$\mathrm{Mo} = \frac{g_z \mu_l^4 \Delta\rho_{gl}}{\rho_l^2 \sigma_{gl}} \qquad \mathrm{Eo} = \frac{g_z \Delta\rho_{gl} d_b^2}{\sigma_{gl}}$$

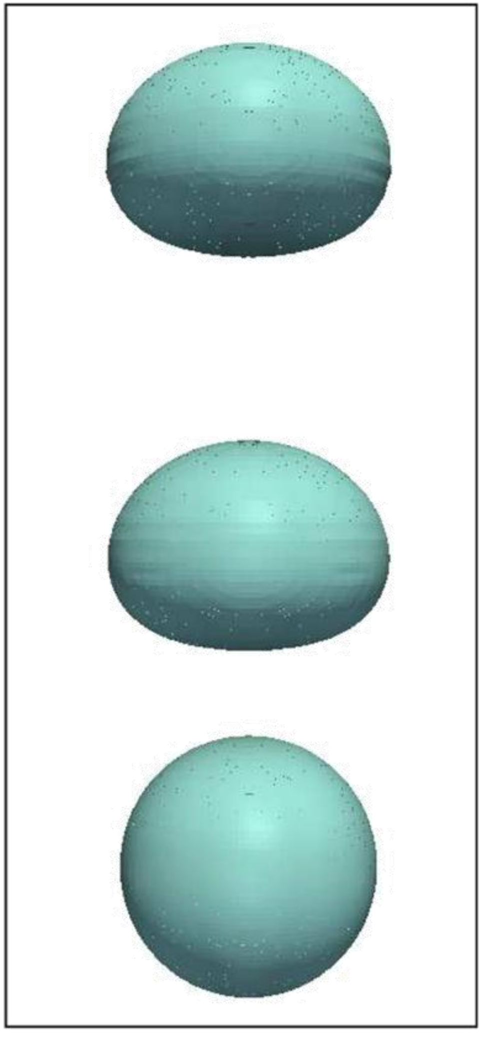
$$\mathrm{Re} = \frac{\rho_l v_\infty d_b}{\mu_l}$$

1) Clift R., Grace J.R., Weber M. *Bubbless, Drops and Particles*. 1978, Academic Press, New York.
2) Annaland M. S., Deen N. G., Kuipers J. A. M., *Numerical simulation of gas bubbles behaviour using a three-dimensional volume of fluid method. Chem. Eng. Sci.,* 2005, 60(11):2999–3011, DOI: 10.1016/j.ces.2005.01.031

Rising bubble – Case B

$\rho_1 : \rho_2 = \mu_1 : \mu_2 = 1{:}100$ Eo=9,71 Mo=0,100

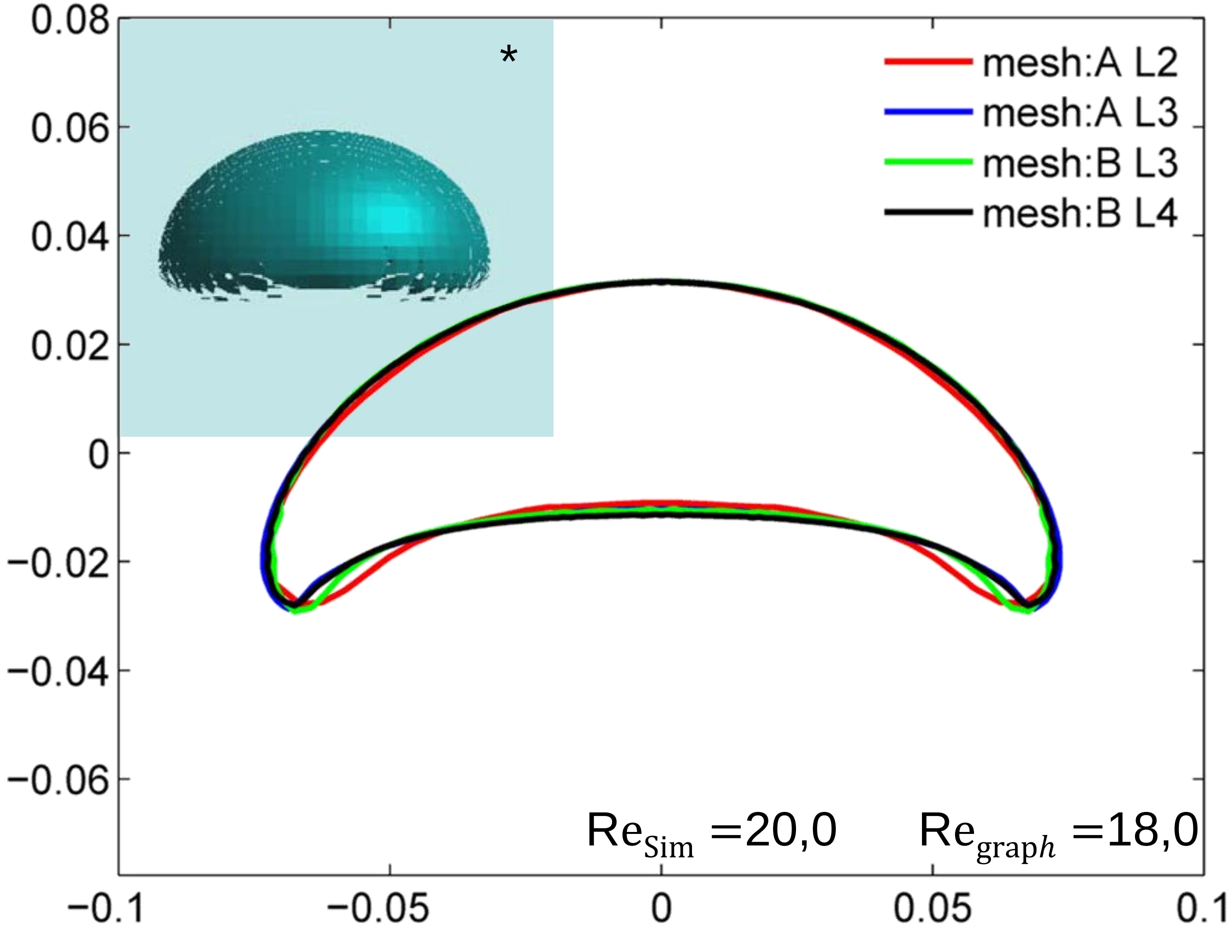


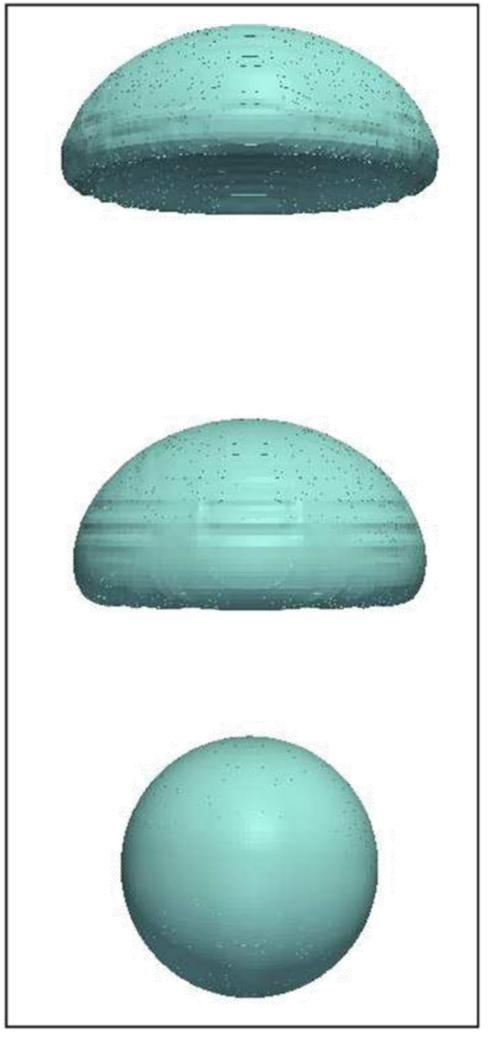


*Annaland M. S., Deen N. G., Kuipers J. A. M., *Numerical simulation of gas bubbles behaviour using a three-dimensional volume of fluid method. Chem. Eng. Sci.,* 2005, 60(11):2999–3011, DOI: 10.1016/j.ces.2005.01.031

Rising bubble – Case C

$\rho_1 : \rho_2 = \mu_1 : \mu_2 = 1:100$ Eo=97,1 Mo=0,971

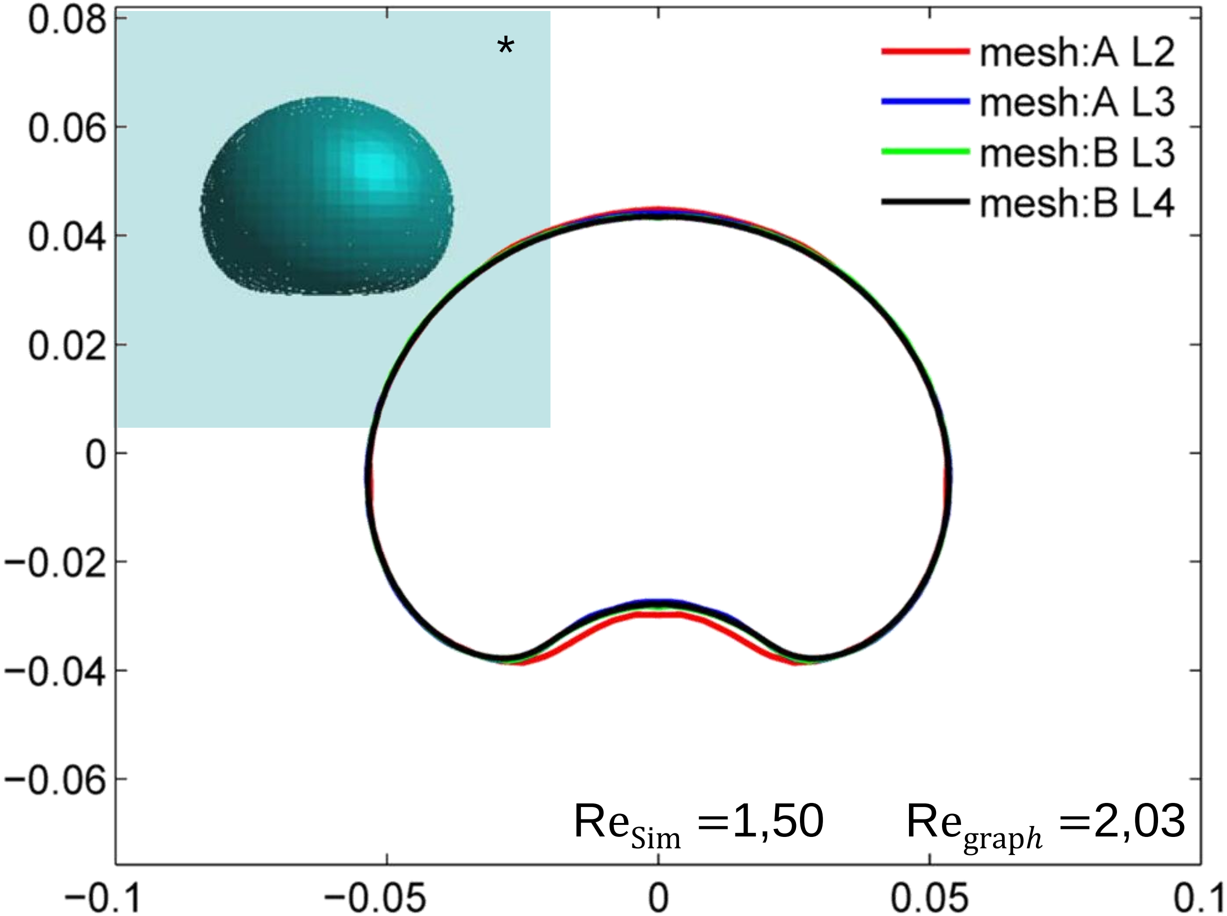


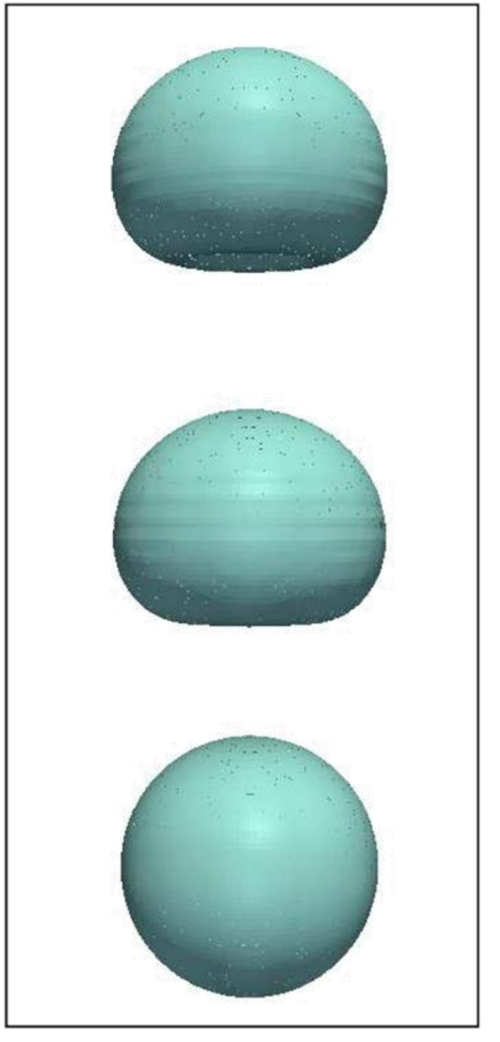


*Annaland M. S., Deen N. G., Kuipers J. A. M., *Numerical simulation of gas bubbles behaviour using a three-dimensional volume of fluid method. Chem. Eng. Sci.,* 2005, 60(11):2999–3011, DOI: 10.1016/j.ces.2005.01.031

Rising bubble – Case D

$\rho_1 : \rho_2 = \mu_1 : \mu_2 = 1{:}100$ Eo=97,1   Mo=1000





*Annaland M. S., Deen N. G., Kuipers J. A. M., *Numerical simulation of gas bubbles behaviour using a three-dimensional volume of fluid method. Chem. Eng. Sci.,* 2005, 60(11):2999–3011, DOI: 10.1016/j.ces.2005.01.031

Benchmarking on experimental results

Continuous phase:

Glucose-Water mixture

$\mu_D = 500 mPa\, s$

$\rho_D = 972\, kg\, m^{-3}$

$\dot{V}_D = 3{,}64\, ml\, min^{-1}$

$\sigma_{CD} = 0{,}034\, N\, m^{-1}$

Silicon oil

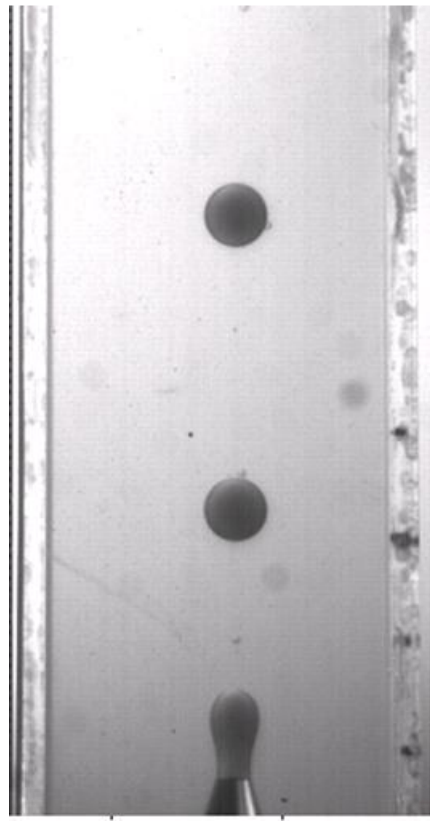
$\mu_C = 500 mPa\, s$

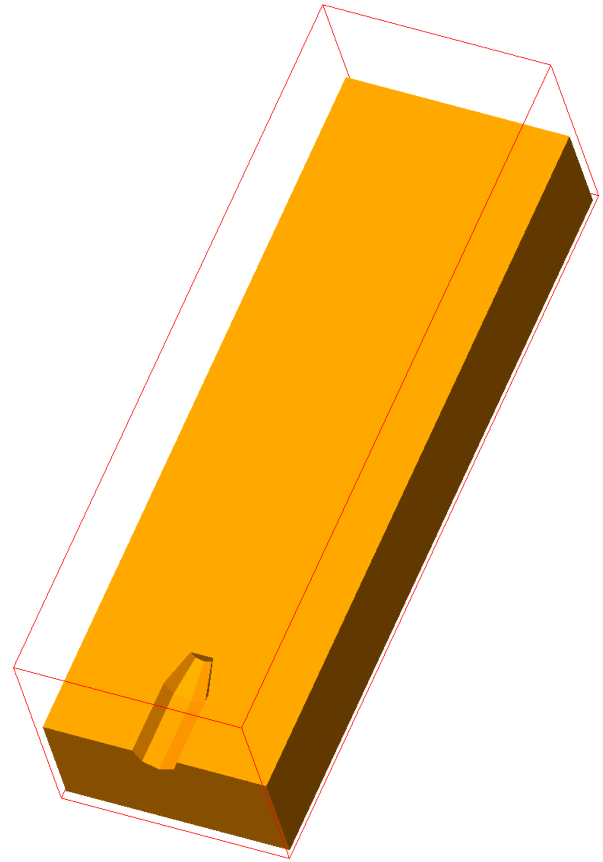
$\rho_C = 1340\, kg\, m^{-3}$

$\dot{V}_C = 99{,}04\, ml min^{-1}$

Dispersed phase:

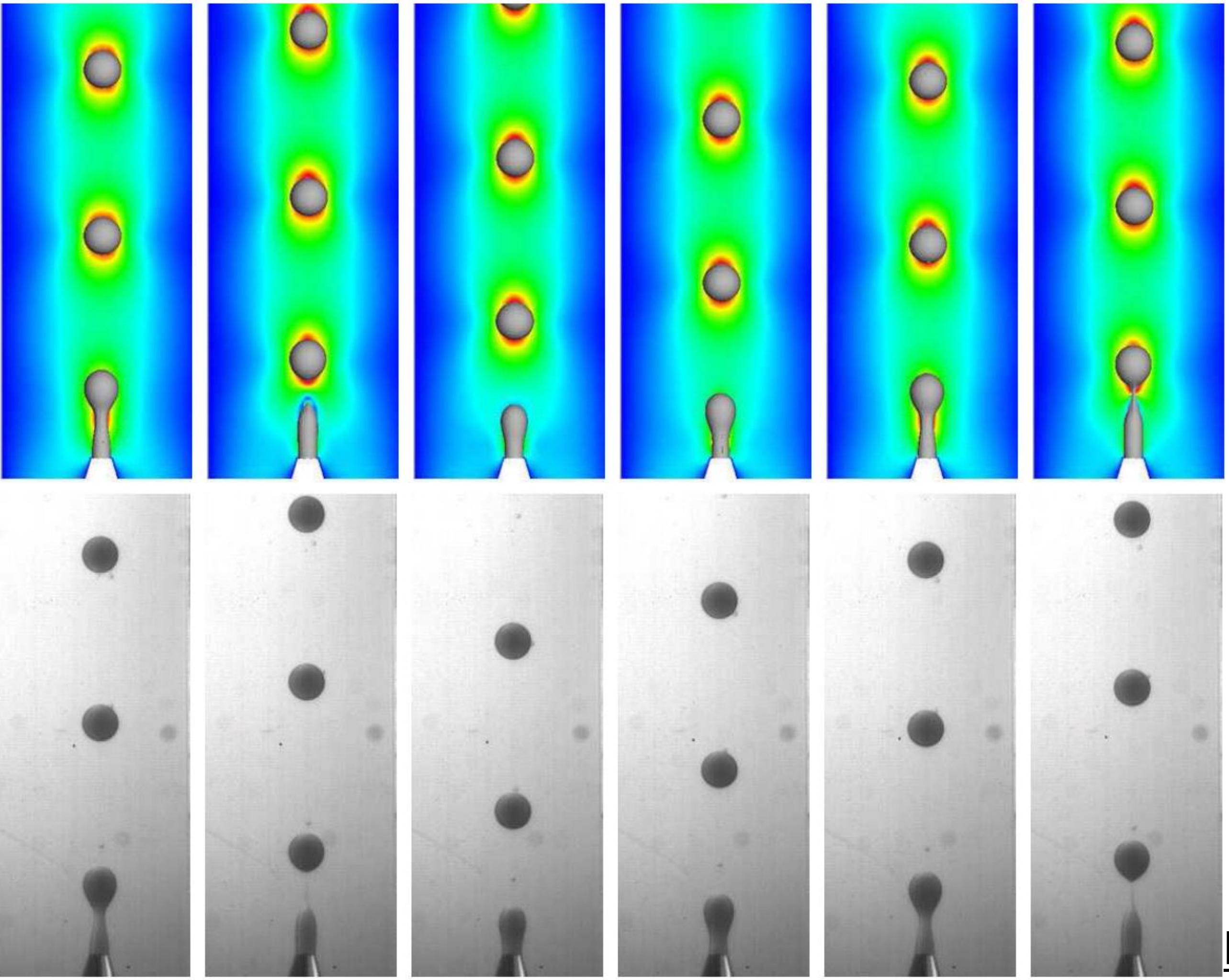
Experimental Set-up with **AG Walzel (BCI/Dortmund)**

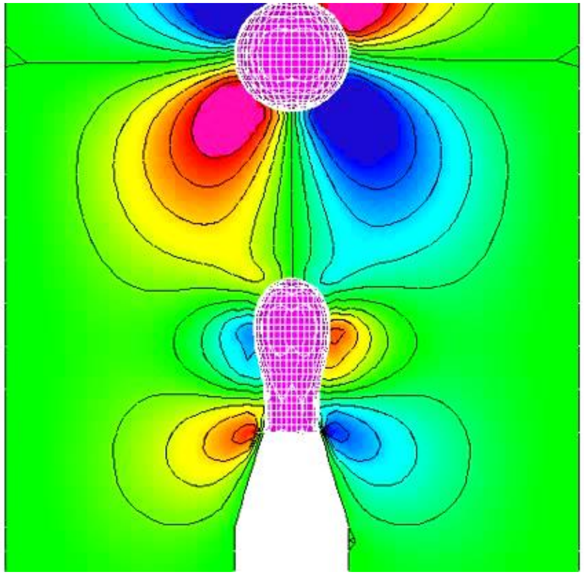




Validation parameters:
- frequency of droplet generation
- droplet size
- stream length

Benchmarking on experimental results



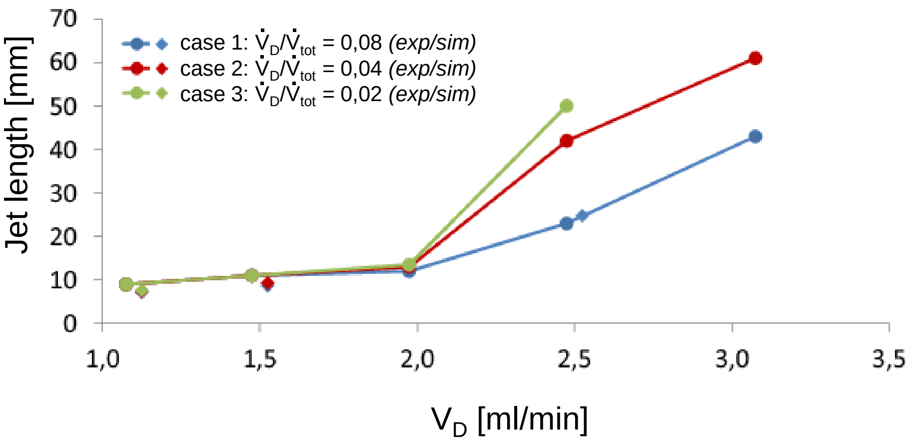


	Separation frequency [Hz]	Droplet size [dm]	Stream Length [dm]
Exp	0,58	0,062	0,122
Sim	0,6	0,058	0,102

Exp. results → Group of Prof. Walzel BCI/Dortmund

Validation for wide range of experiments

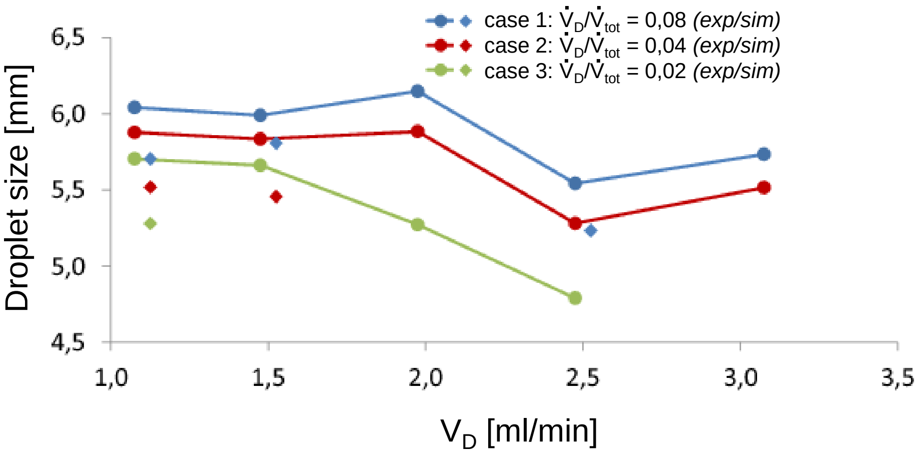
Experimental results: Group of Prof. Walzel BCI/Dortmund



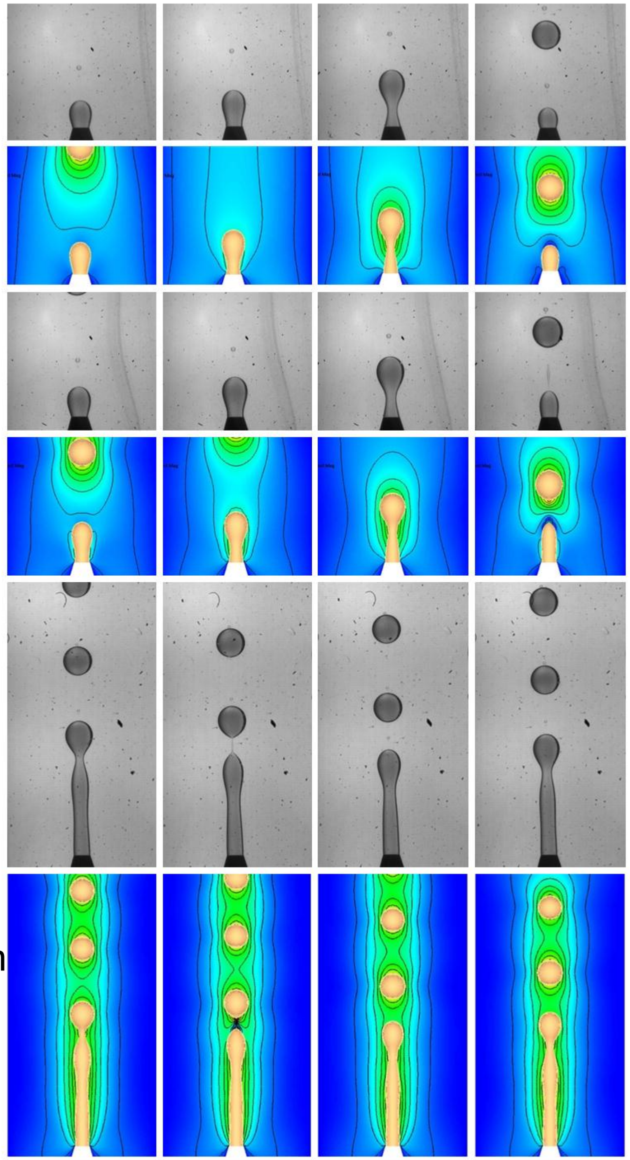
Example 1:
$\dot{V}_D$= 1,1 ml/min
$\dot{V}_C$= 13,0 ml/min
$\dot{V}_D/\dot{V}_{tot}$ = 0,08

Example 2:
$\dot{V}_D$= 1,5 ml/min
$\dot{V}_C$= 41,1 ml/min
$\dot{V}_D/\dot{V}_{tot}$ = 0,04

Effects of contact angle?



Example 3:
$\dot{V}_D$= 2,5 ml/min
$\dot{V}_C$= 123,2 ml/min
$\dot{V}_D/\dot{V}_{tot}$ = 0,02



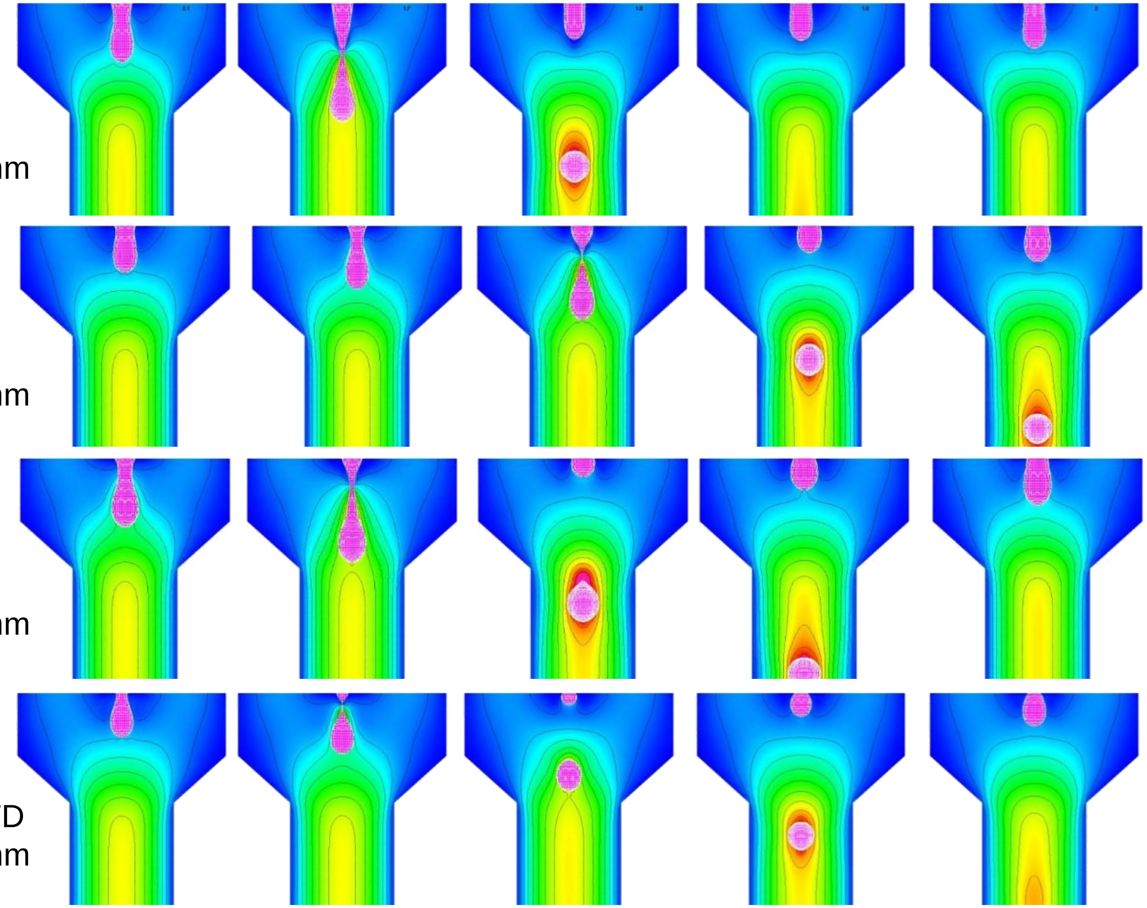
Influence of modulation

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

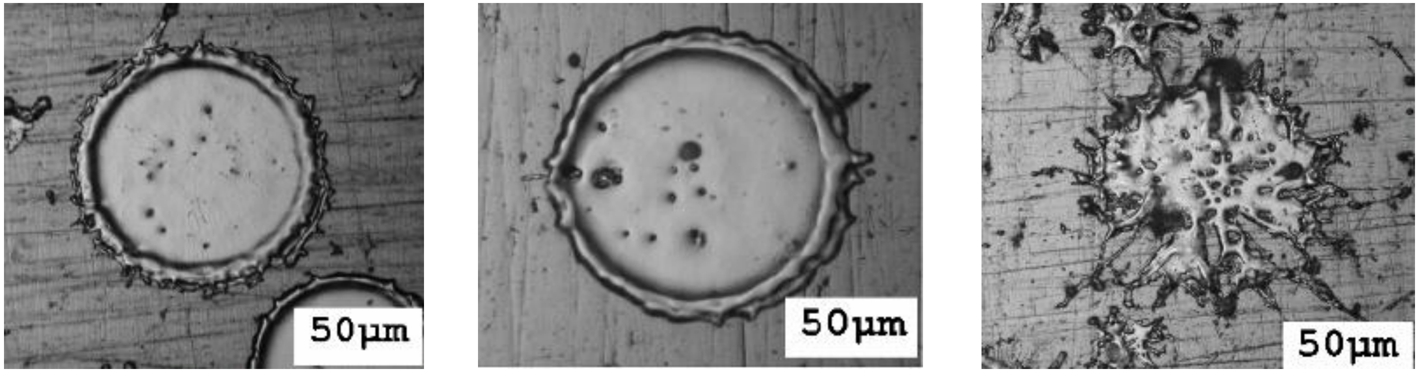
Regulated
Flowrate: 75%
Capillary: 50% STD
Droplet size: 4.5mm



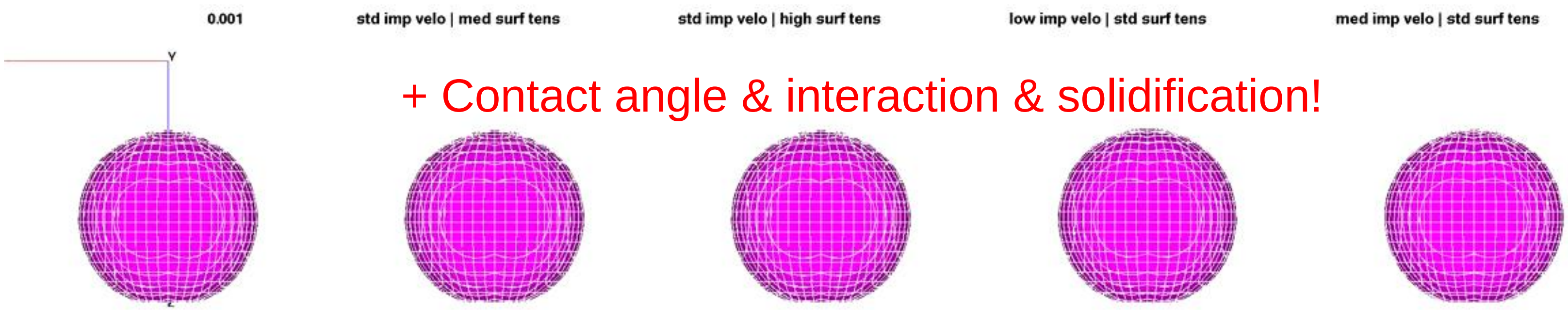
Resulting operation envelope:

- Size: 4.5 mm – 5.7 mm
- Volume: 0.38 cm^3 – 0.77 cm^3

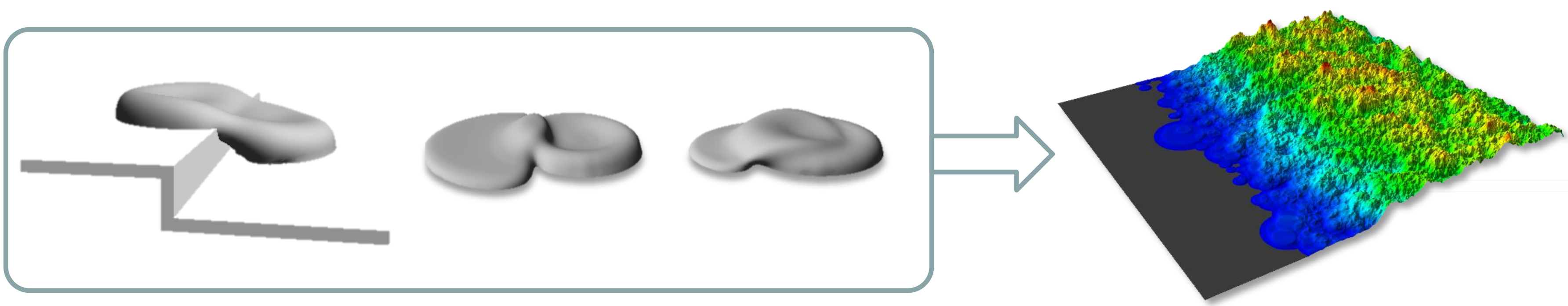
Droplet deposition



Pourmousa A, *WIRE-ARC SPRAYING SYSTEM: Particle Production, Transport, and Deposition*, Department of Mechanical and Industrial Engineering University of Toronto, PhD Thesis, 2007.



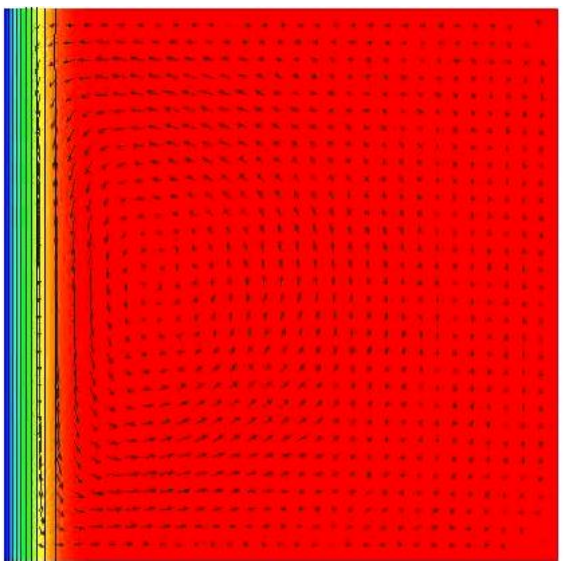
+ Contact angle & interaction & solidification!



Solidification

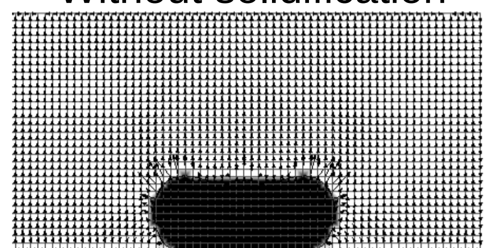
$$\rho c_p\left(\frac{\partial\Theta}{\partial t}+\mathbf{v}\cdot\nabla\Theta\right)-\nabla\cdot(k\nabla\Theta)=\rho g(\Theta) \quad \overset{f}{\Longrightarrow} \quad H_L(\Theta)=\begin{cases} L, & \Theta>\Theta_L \\ L\dfrac{\Theta-\Theta_s}{\Theta_L-\Theta_s}, & \Theta_s\le\Theta<\Theta_L \\ 0, & \Theta<\Theta_s \end{cases}$$

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

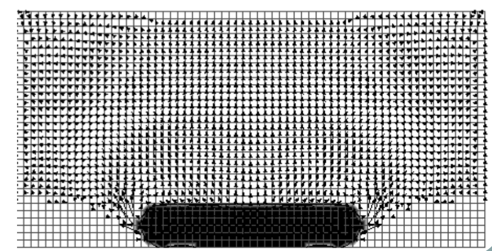


Influence on impinging droplets

Without solidification



With solidification



1) Swaminathan C. R., Voller V., *On the enthalpy method,* Int. J. Num. Meth. Heat Fluid Flow, 1993, **3**, 233-244.
2) McDaniel D. J., Zabaras N., *A Least squares front tracking FEM analysis of phase change with natural convection,* Int. J. for Num. Meth. In Eng., 1994, **37**, 2755-2777.

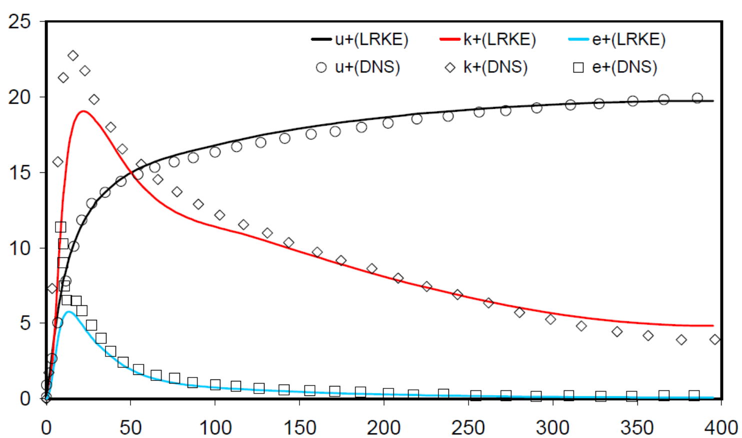
Validation of turbulence models

- Standard k-ε model
- Chien's low Re k-ε model

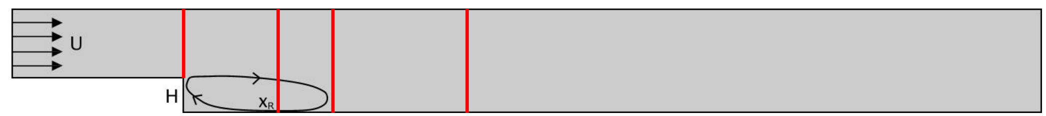
+ Boundary conditions!

Channel flow for $\mathrm{Re}_\tau = \dfrac{du_\tau}{\nu} = 395$

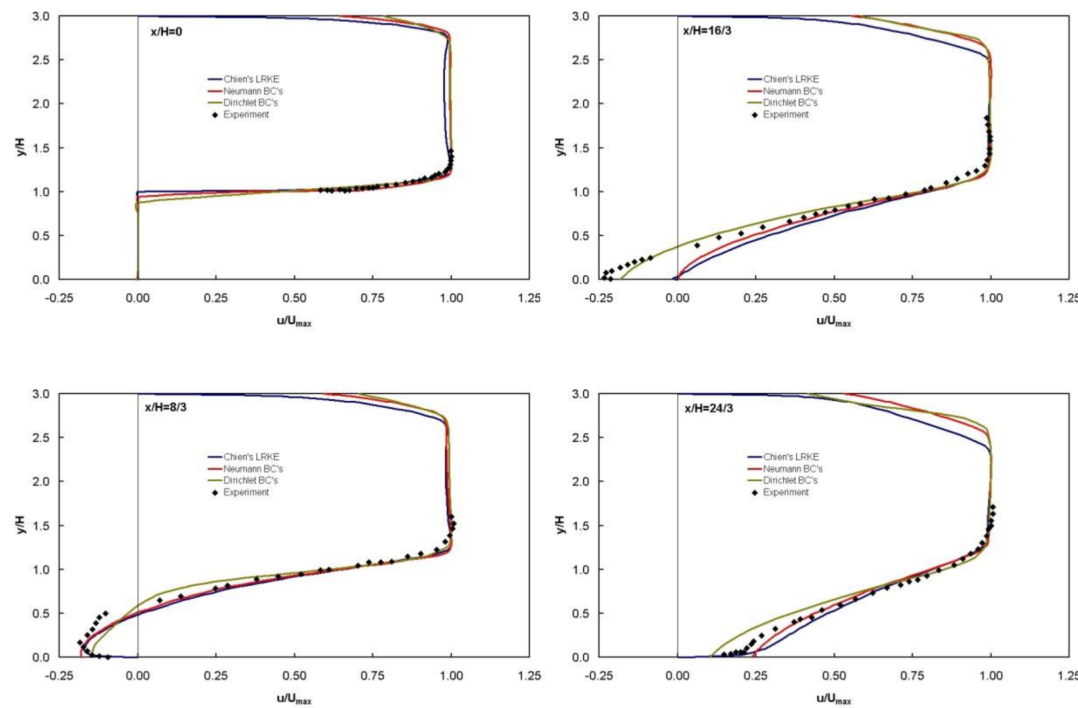
$$y^+ = \frac{u_\tau y}{\nu}, \quad u^+ = \frac{u_x}{u_\tau}, \quad k^+ = \frac{k}{u_\tau^2}, \quad \varepsilon^+ = \frac{\varepsilon \nu}{u_\tau^4}$$



Backward facing step for $\mathrm{Re}_\tau = \dfrac{HU}{\nu} = 47{,}625$



Reattachment length $5.0 < x_{r,\mathrm{literature}} < 6.5$



Conclusions and future plans

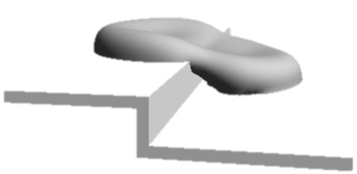
Overview of the modules of the desired simulation tool

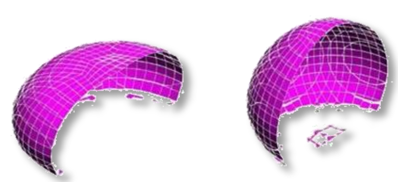
module:	status:
CFD solver	Parallelized, multi-grid based, high order, Benchmarked
Level Set	Parallelized and equipped with reinitialization, Benchmarked
Heat equation	Parallelized, Solidification is tested and verified in 2D
Turbulence model	Sequential, tested and verified in 3D, low/high Reynolds number extensions

Dynamics of droplet deposition

CFD solver / Level Set + Heat equation

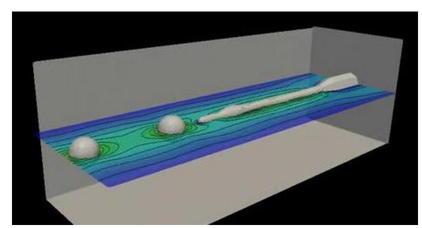
+ Solidification

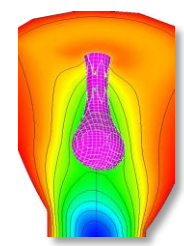




Dynamics of droplet generation

CFD solver / Level Set + Turbulence model





+ Modulation

+ Experimental/computational reference results ⇨ Proposal of benchmark problems