CFD simulation of monodisperse droplet generation by means of jet break-up

DFG – SPP 1423 „Prozess-Spray“

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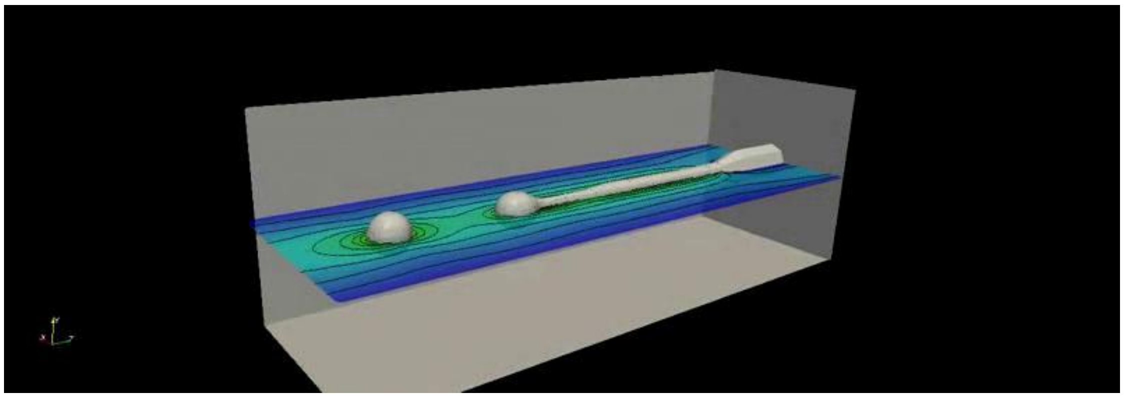
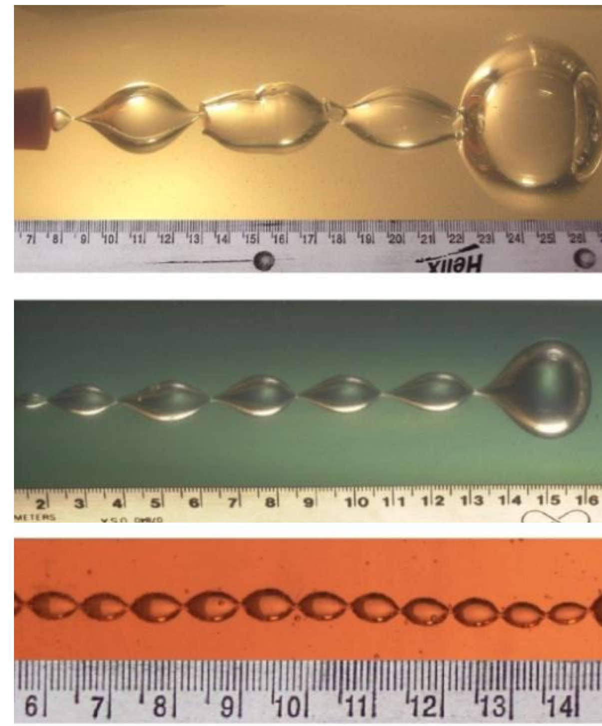
Motivation and Goals

CFD simulation tool: *Controlled droplet generation in jets*
Simulation results: *dispersity, droplet generation frequency, jet length*
Simulation parameters: *physical parameters, rheological properties, modulation parameters*

1) Jetting simulations with Newtonian fluids



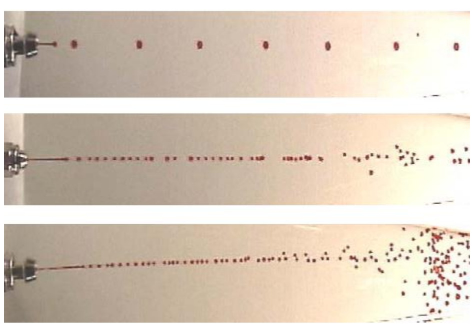
2) Non-Newtonian fluids …



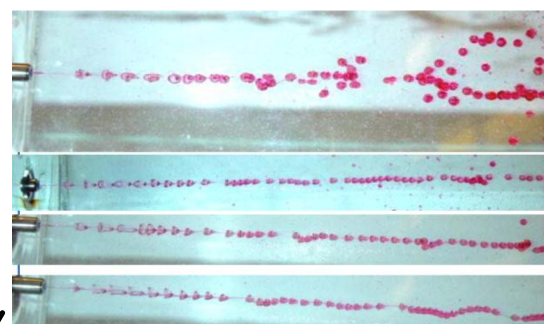
Chhabra: Bubbles, Drops and Particles in Non-Newtonian Fluids

3) Modulation analysis of jetting simulations

Increasing pressure



Increasing puls. freq.



2005 NOVA Chemicals Corporation

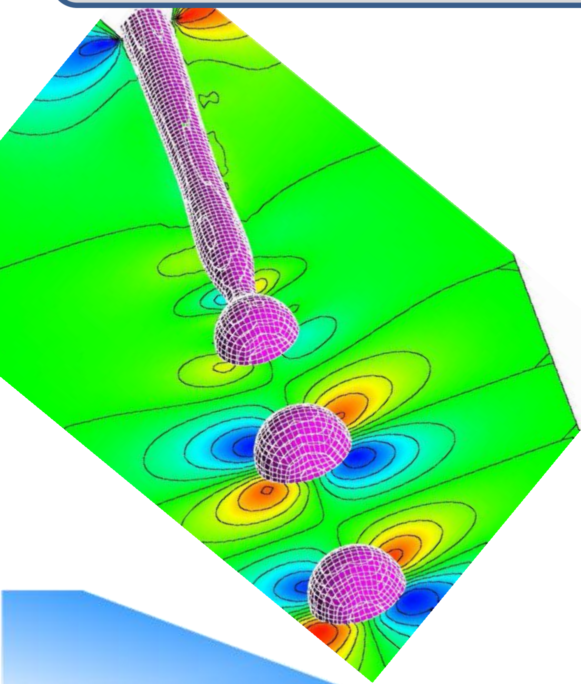
Methods

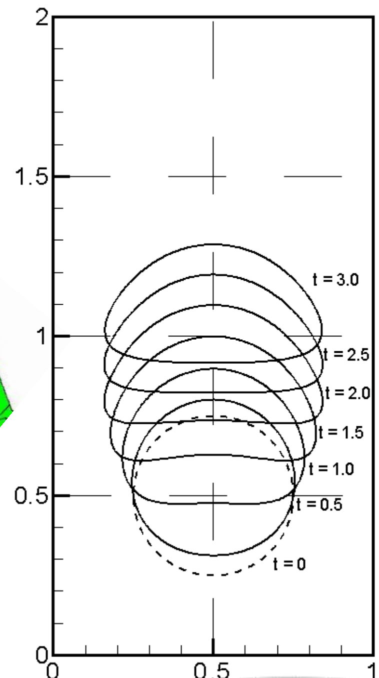
- Mass conservative FEM levelset approach with „exact“ interphase reconstruction. Implicit treatment of the surface tension force term

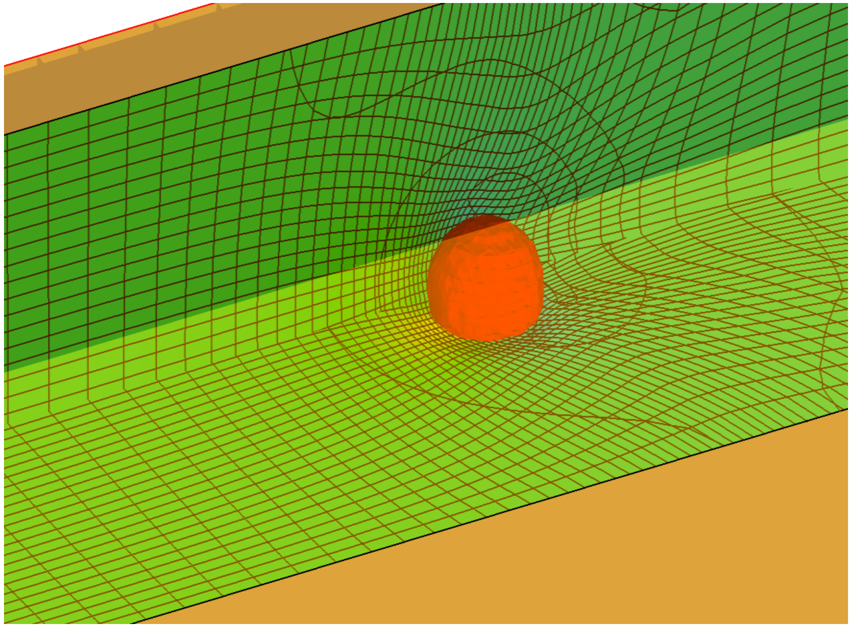
- Fast solvers (parallel multigrid) for scalar equations and for the Pressure-Poisson equation supporting large density jumps

- Systematic validation and benchmarking (CFX, FEMLAB, FLUENT, OpenFOAM).

- Incorporation of adaptive grid deformation techniques (ALE approach)







Governing Equations

The incompressible Navier Stokes equation

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

$$\nabla\cdot\mathbf{v} = 0$$

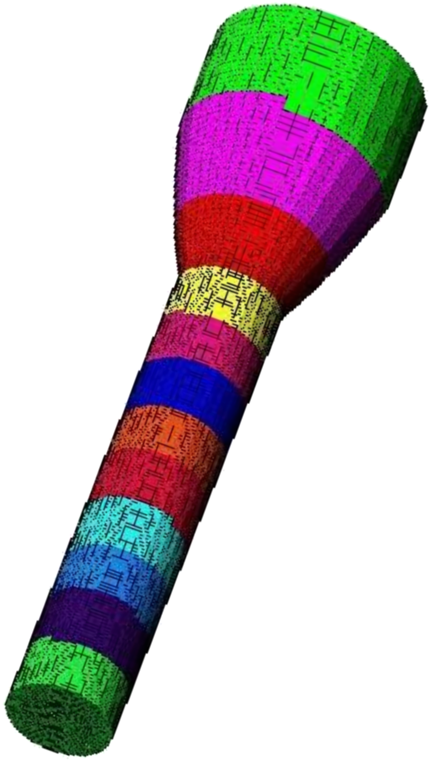
Interphase tension force

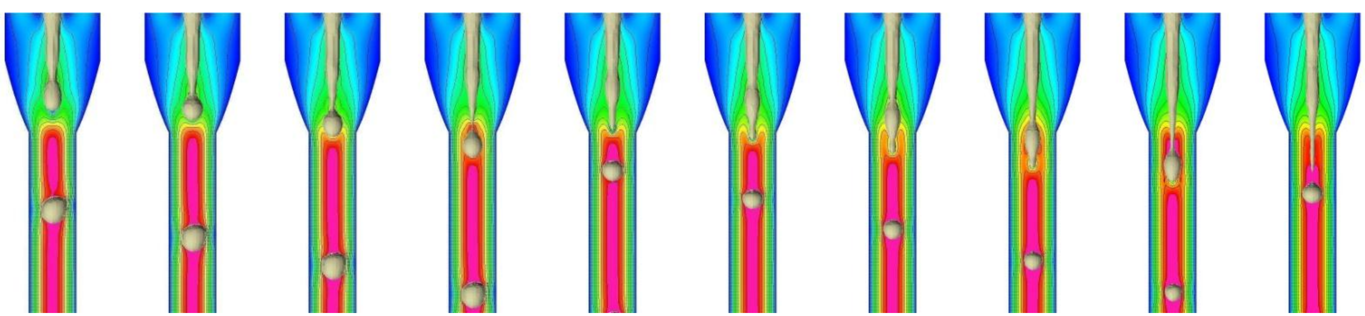
$$\mathbf{f}_{ST} = \sigma\kappa\mathbf{n}, \quad \kappa = -\nabla\cdot\mathbf{n} \quad \text{on} \quad \Gamma$$

unknown interphase location

Dependency of physical quantities

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

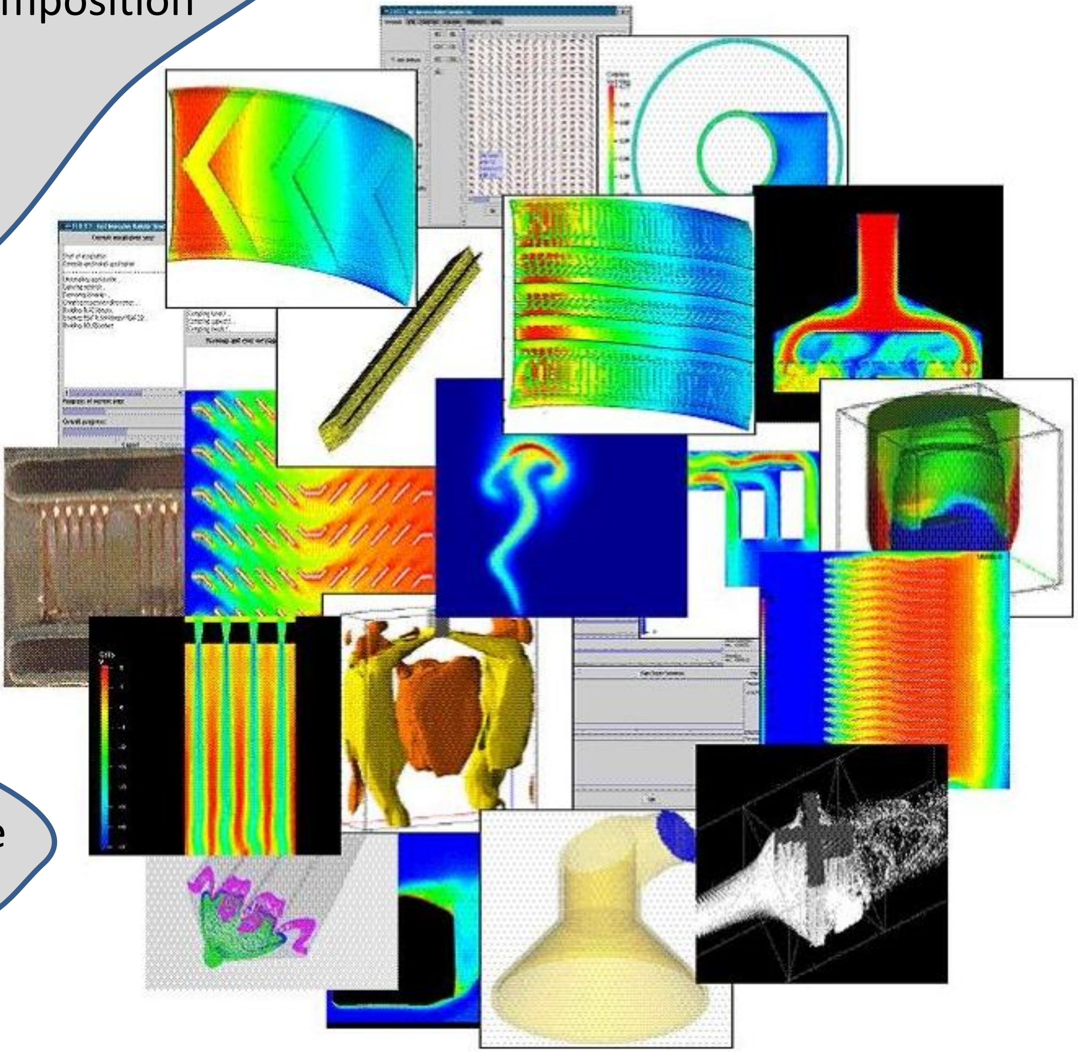




Efficient Flow Solver

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



Discretization:

- Navier-Stokes: FEM Q_2/P_1
- Level Set: DG-FEM P_1

in space

- Crank-Nicholson scheme in time

Efficient Interphase Capturing

Level Set Method (→"smooth" distance function)

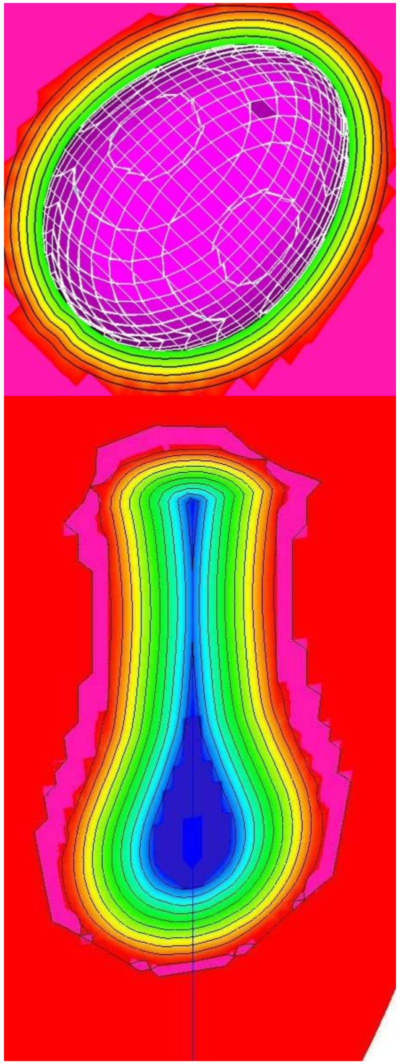
$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0$$

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

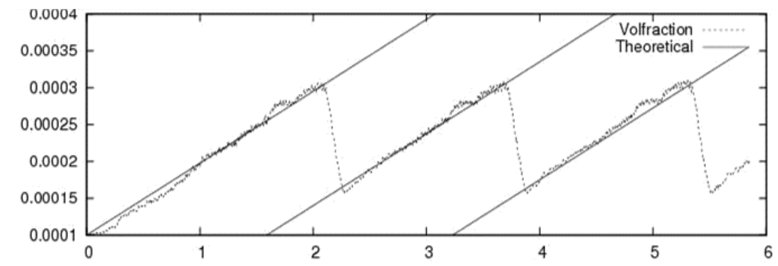
- **Steep gradients** of physical quantities at the interphase
- **Reinitialization** (smoothed sign function, artificial movement of the interphase)
- **Mass conservation** (during advection and reinitialization of the Level Set function)
- Representation of **interphacial tension**: CSF, Line Integral,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

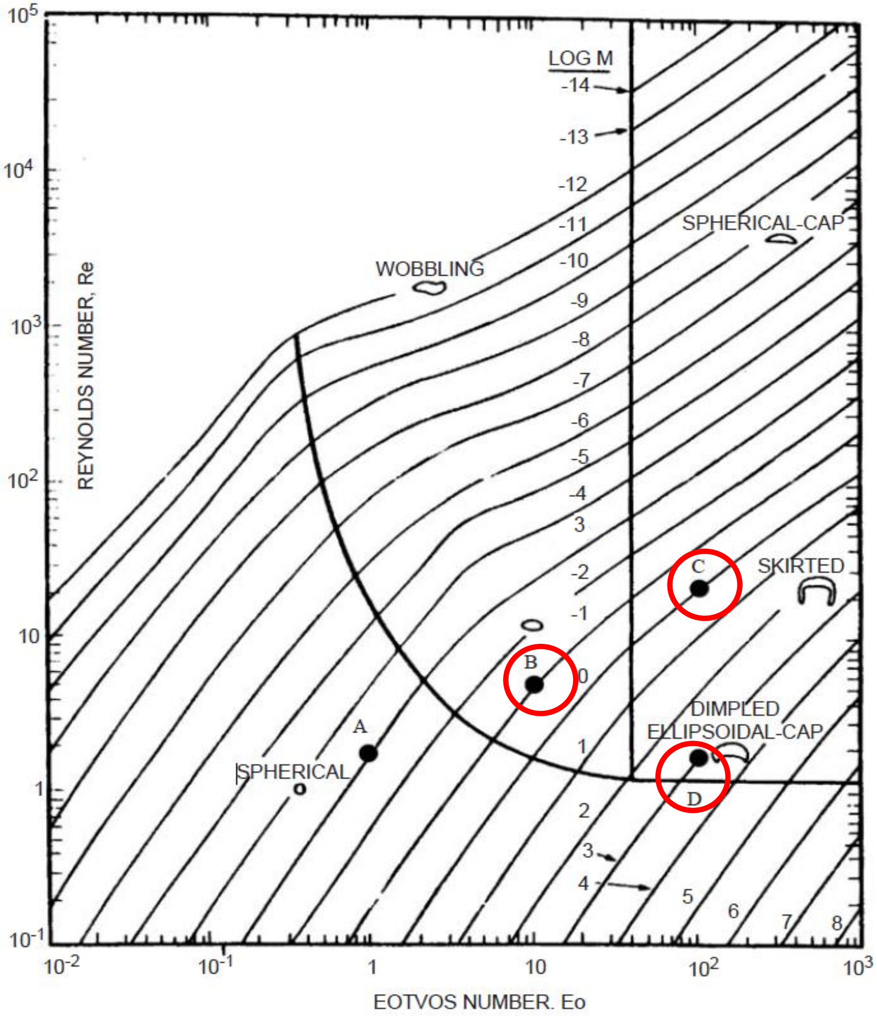
$$\frac{\partial \phi}{\partial \tau} + \mathbf{u}\cdot\nabla\phi = S(\phi) \qquad \mathbf{u} = S(\phi)\frac{\nabla\phi}{|\nabla\phi|} \quad \Leftrightarrow \quad |\nabla\phi| = 1$$

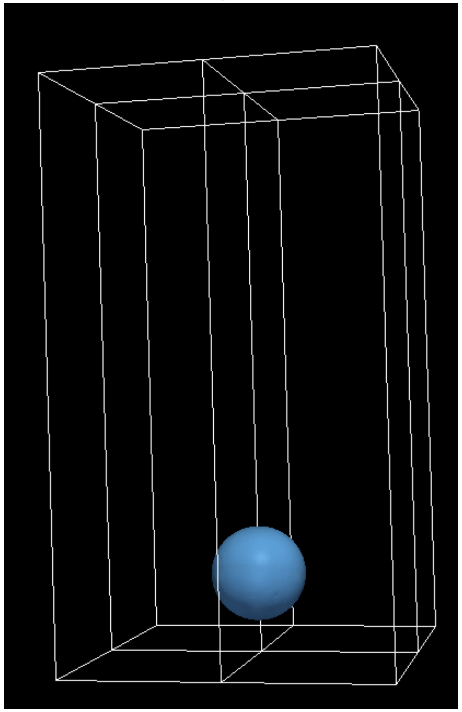


CSF smoothening with Dirac δ function

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

Validation for the rising bubble problem





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

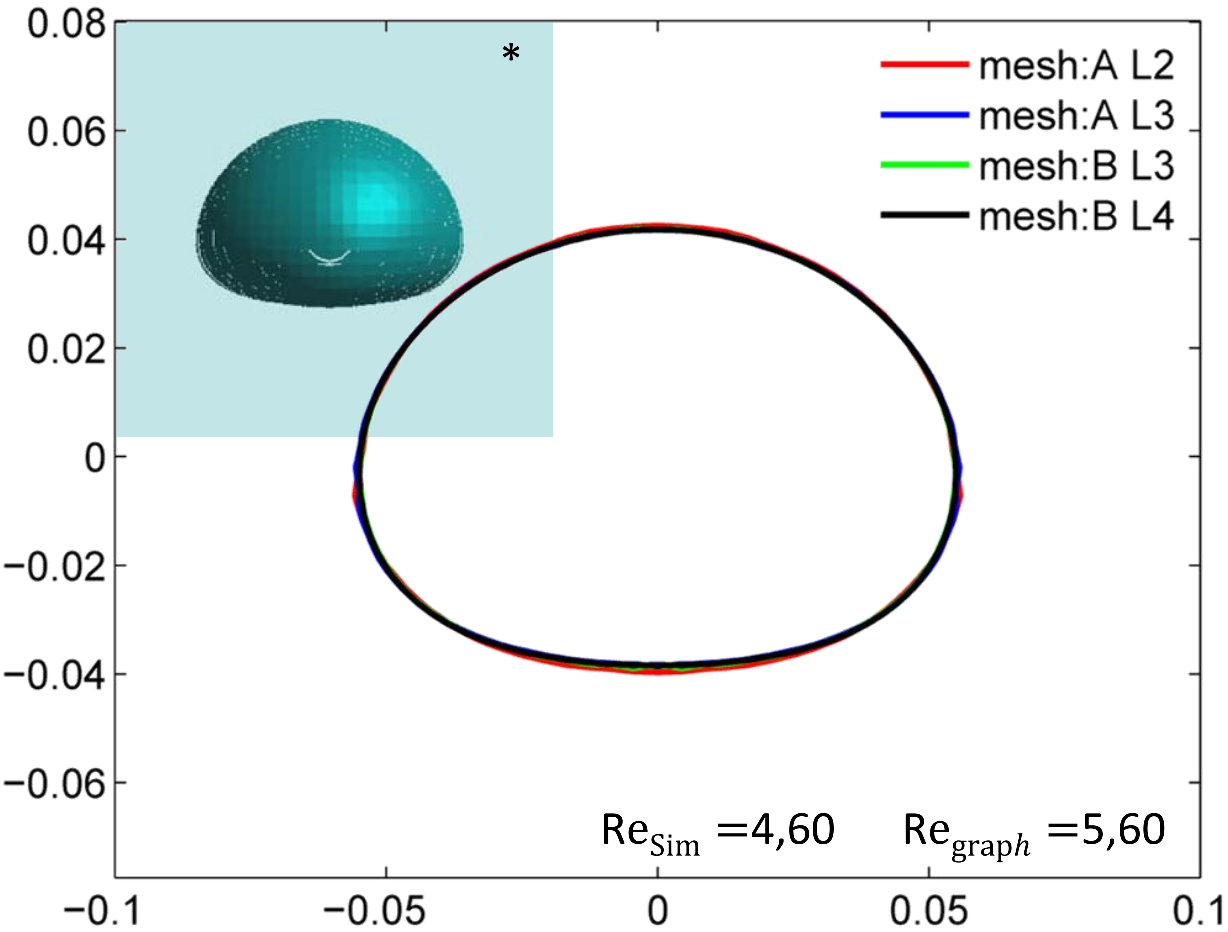
$$\mathrm{Mo} = \frac{g_z \mu_l^4 \Delta\rho_{gl}}{\rho_l^2 \sigma_{gl}} \qquad \mathrm{Eo} = \frac{g_z \Delta\rho_{gl} d_b^2}{\sigma_{gl}}$$

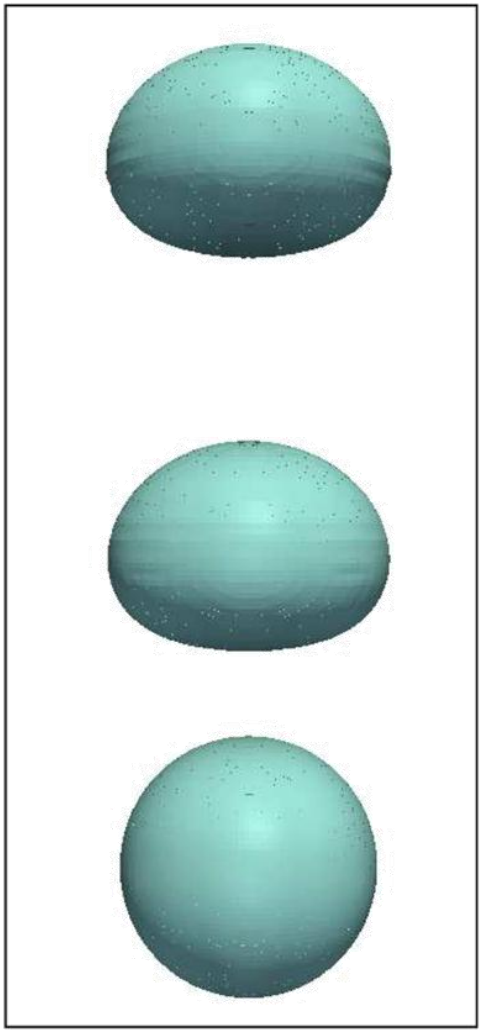
$$\mathrm{Re} = \frac{\rho_l v_\infty d_b}{\mu_l}$$

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

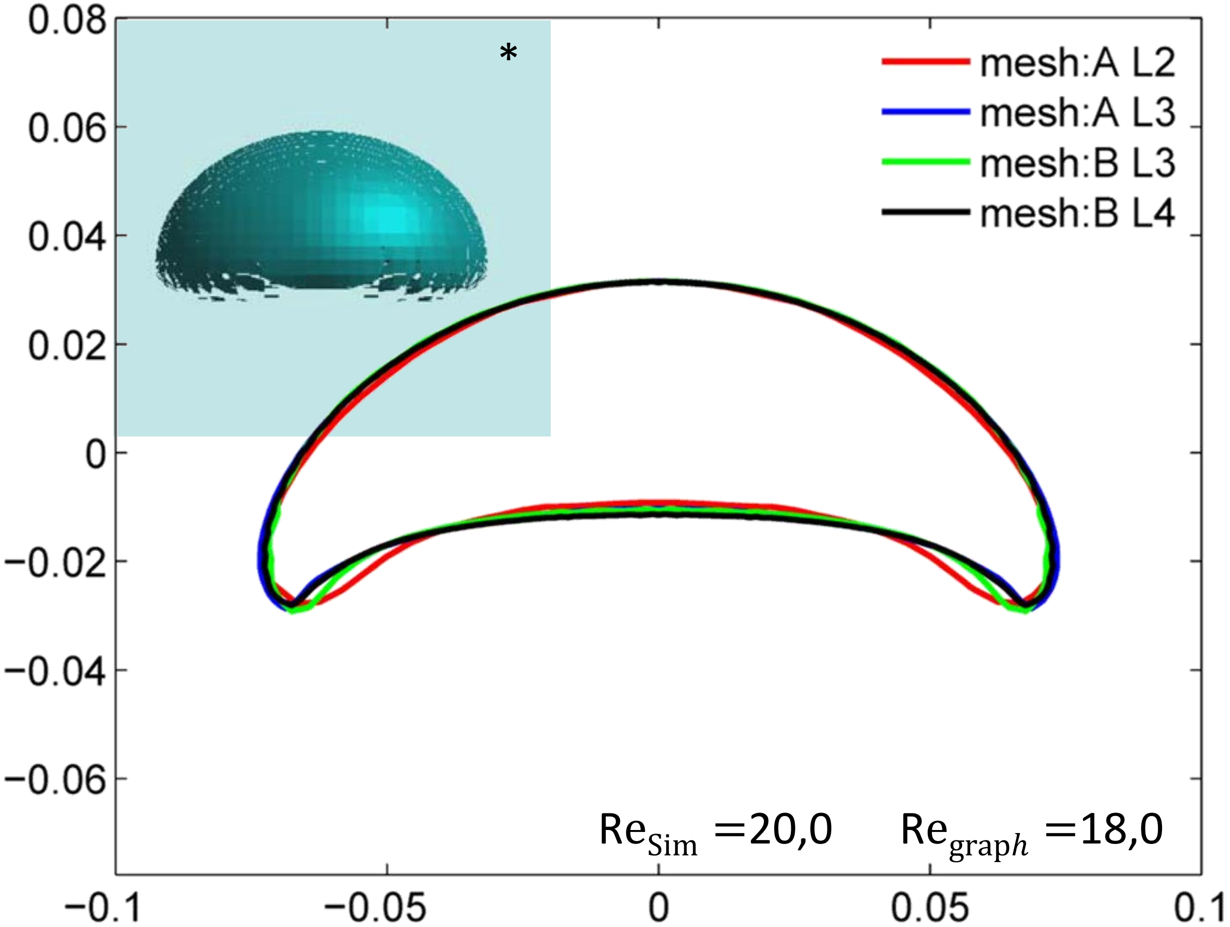


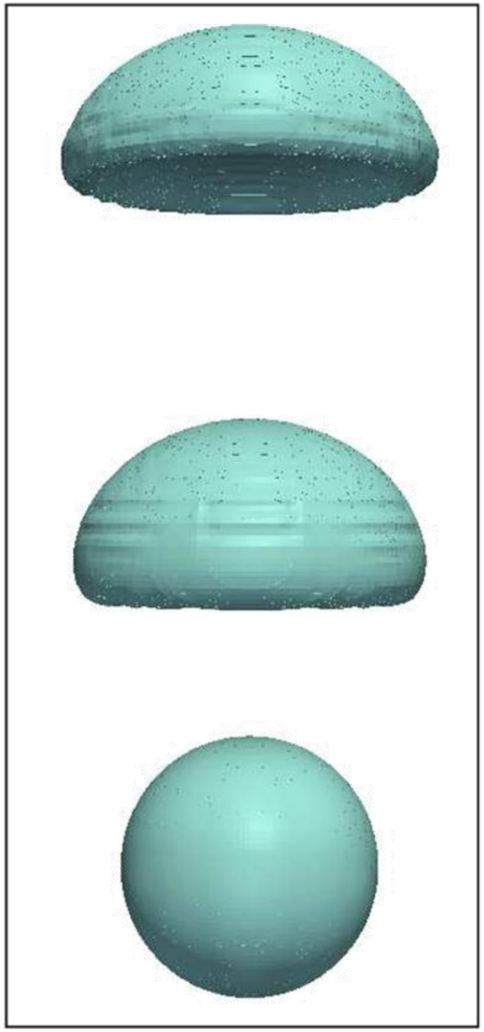


*Annaland M. S., Deen N. G., Kuipers J. A. M., *Numerical simulation of gas bubbles behaviour using a three-dimensional volume of fluid method. Chem. Eng. Sci.*, 2005, 60(11):2999–3011, DOI: 10.1016/j.ces.2005.01.031

Rising bubble – Case C

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

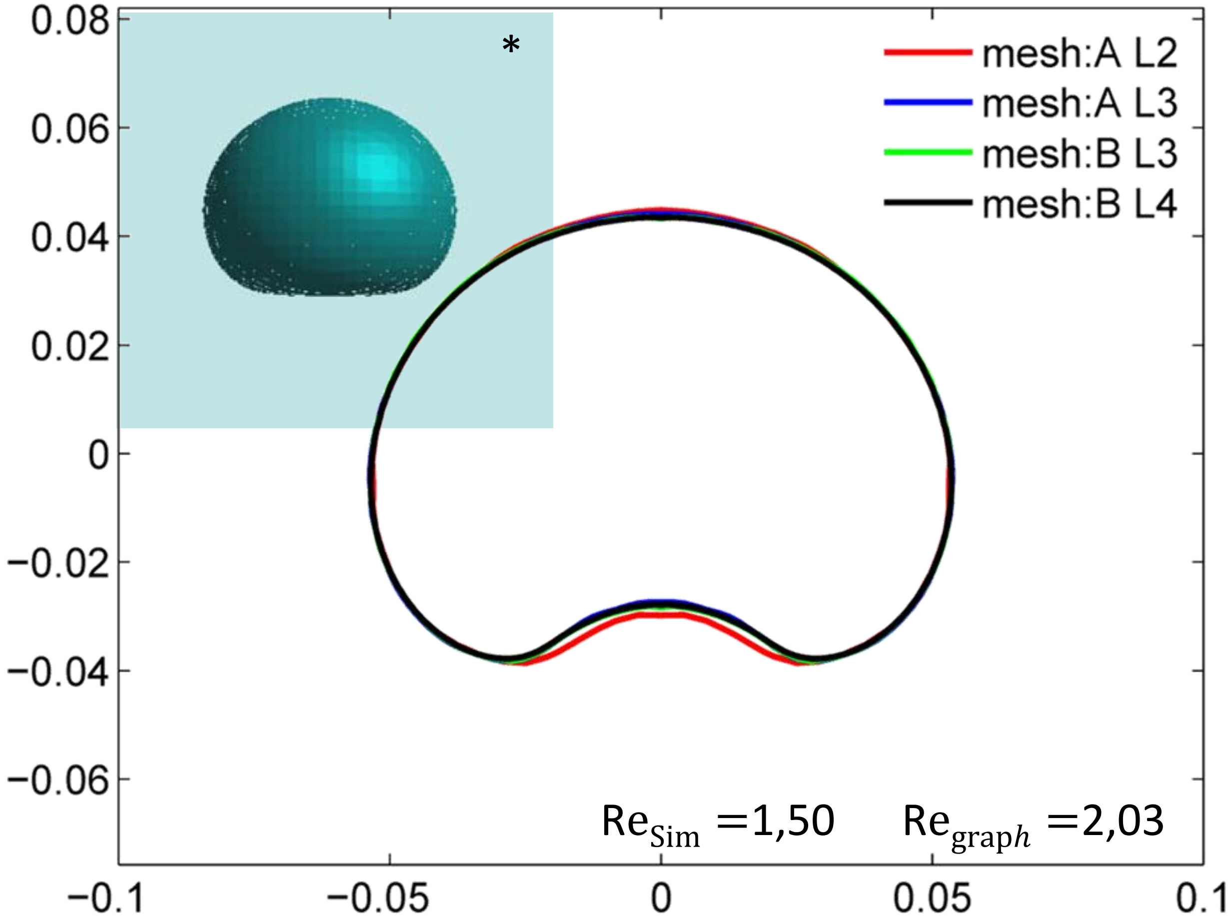


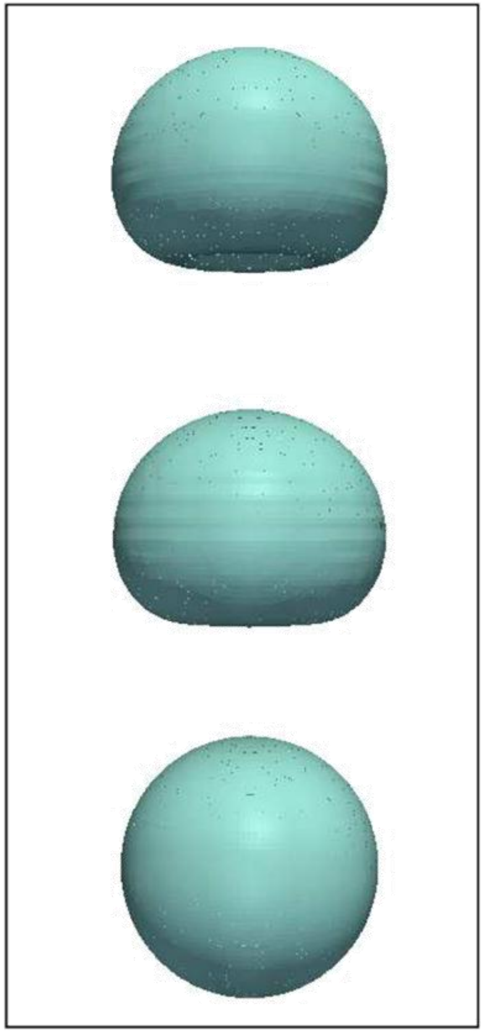


*Annaland M. S., Deen N. G., Kuipers J. A. M., *Numerical simulation of gas bubbles behaviour using a three-dimensional volume of fluid method. Chem. Eng. Sci.,* 2005, 60(11):2999–3011, DOI: 10.1016/j.ces.2005.01.031

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

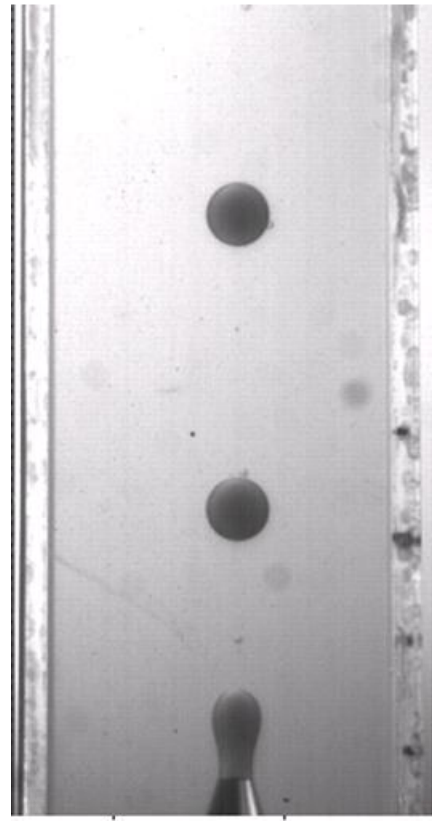
$\mu_C = 500\, mPa\, s$

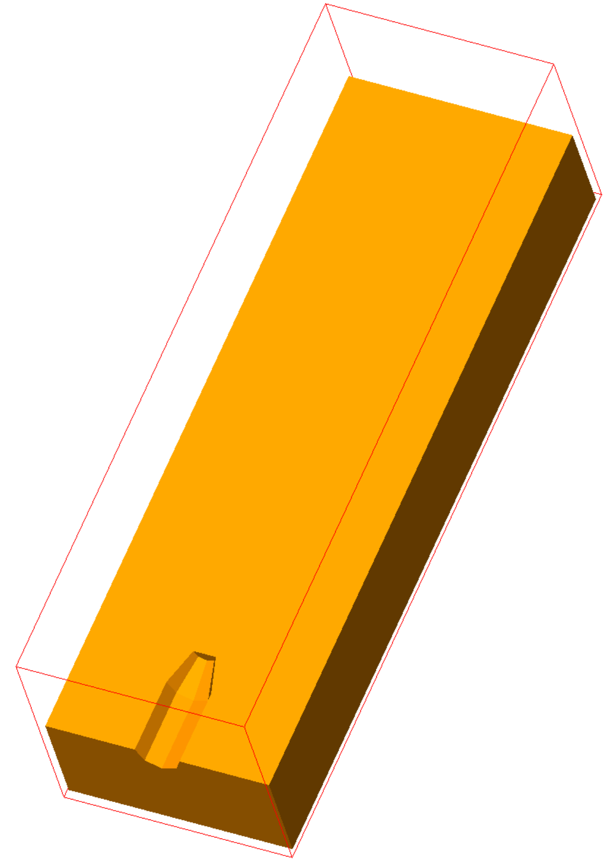
$\rho_C = 1340\, kg\, m^{-3}$

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

Dispersed phase:

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

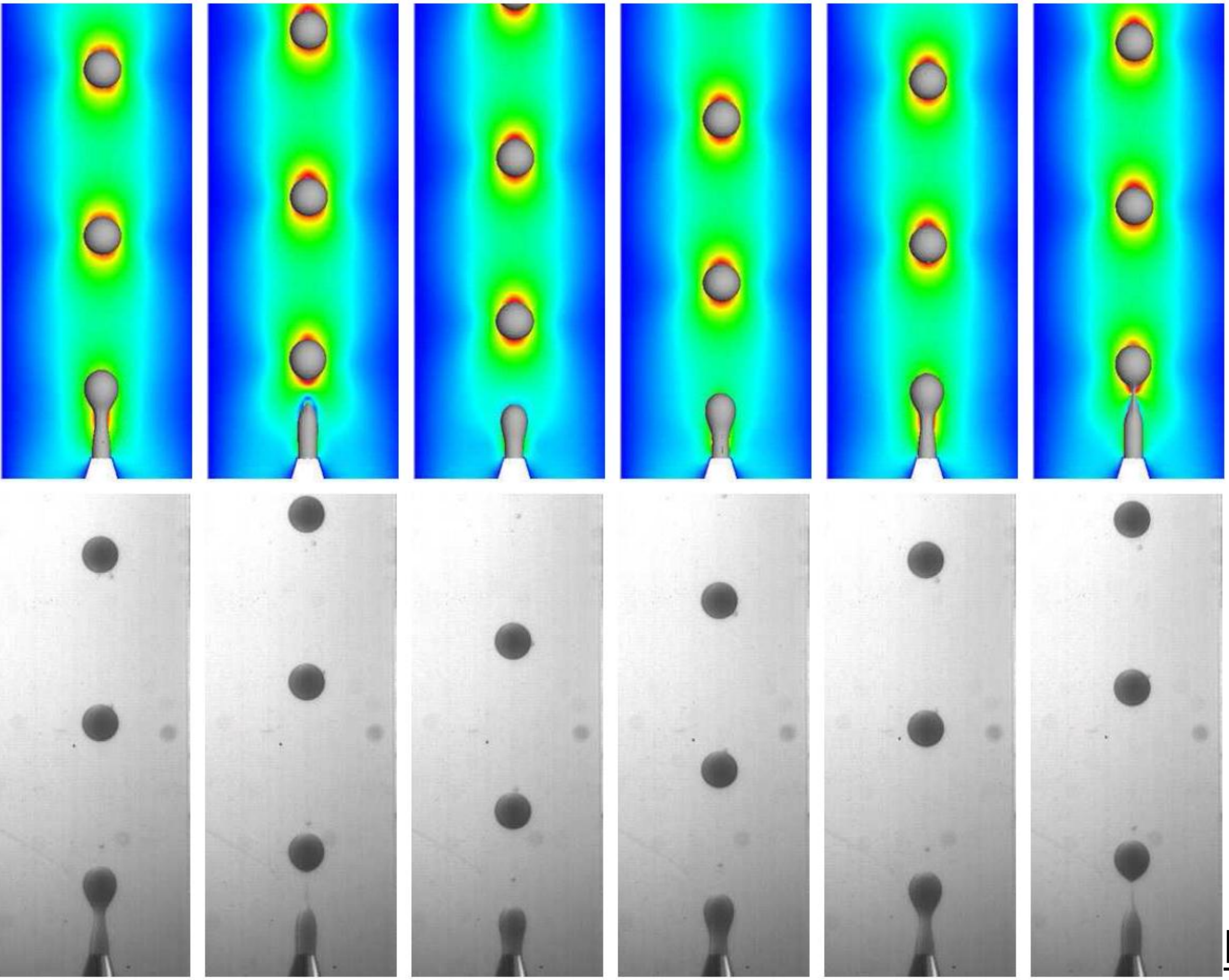


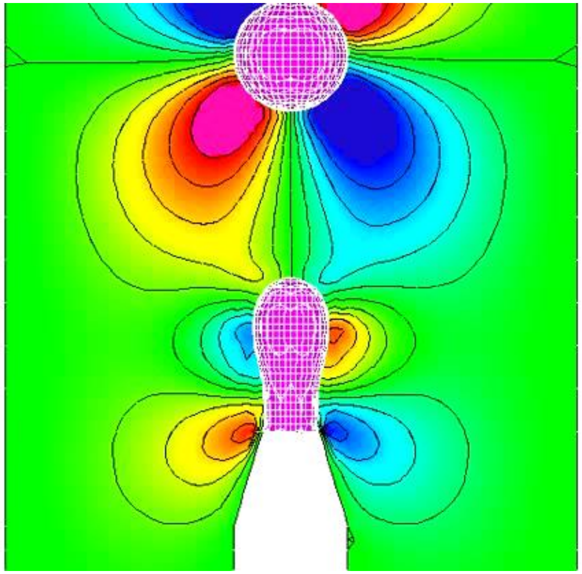


Validation parameters:

- frequency of droplet generation
- droplet size
- stream length

Benchmarking on experimental results



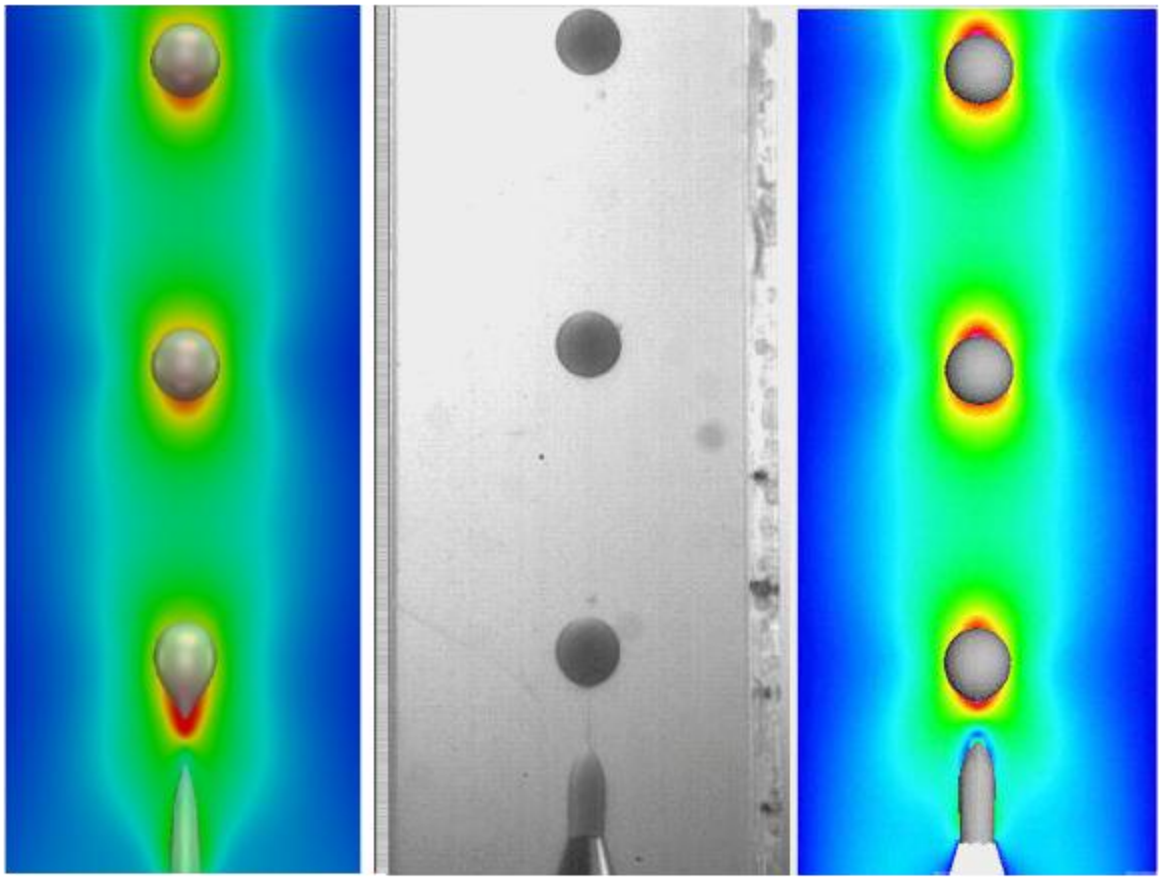


	Separation frequency [Hz]	Droplet size [dm]	Stream Length [dm]
Exp	0,58	0,062	0,122
Sim	0,6	0,058	0,102

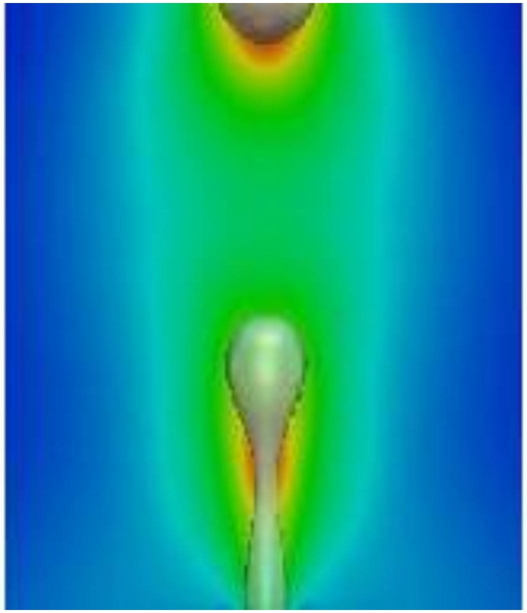
Exp. results → Group of Prof. Walzel BCI/Dortmund

Benchmarking on experimental results

iRMB - **Ying Wang,** Institute for Computational Modeling in Civil Engineering, TU Braunschweig Mühlen-pfordtstraße 4-5 D-38106, Braunschweig, Germany



iRMB - LB | Exp | TU Do - FEM

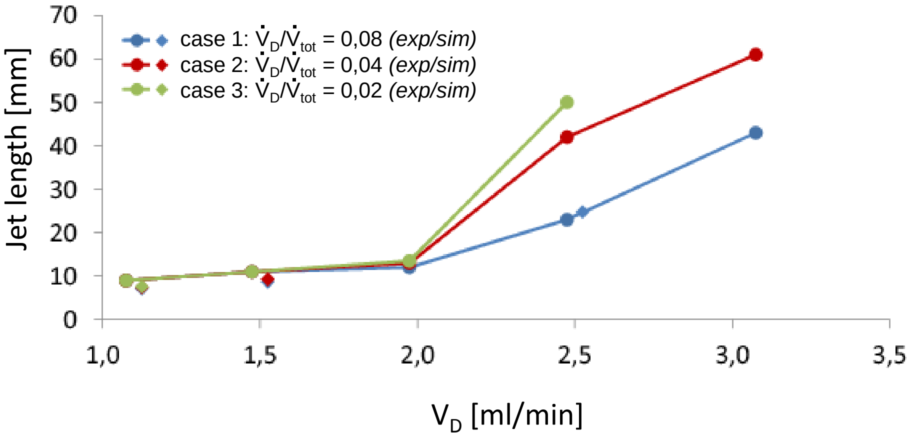


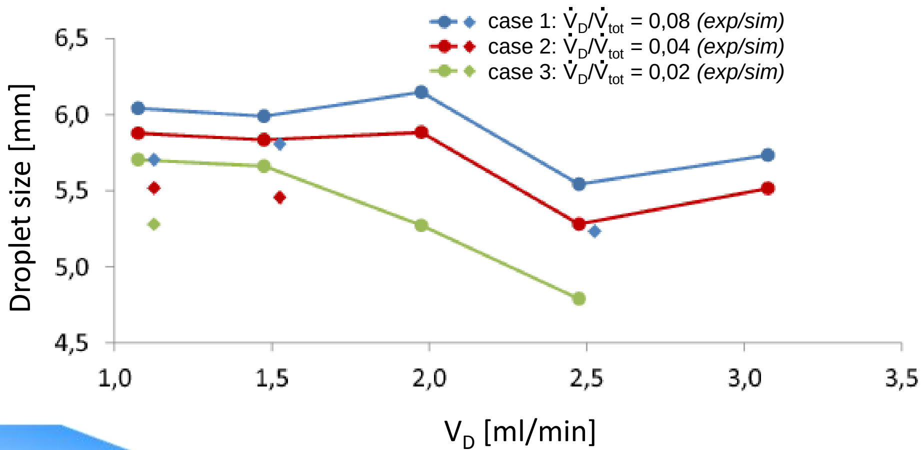
	Separation frequency [Hz]	Droplet size [dm]	Stream Length [dm]
Exp	0,58	0,062	0,122
Sim	0,37	0,068	0,113

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

Validation for wide range of experiments

Experimental results: Group of Prof. Walzel BCI/Dortmund



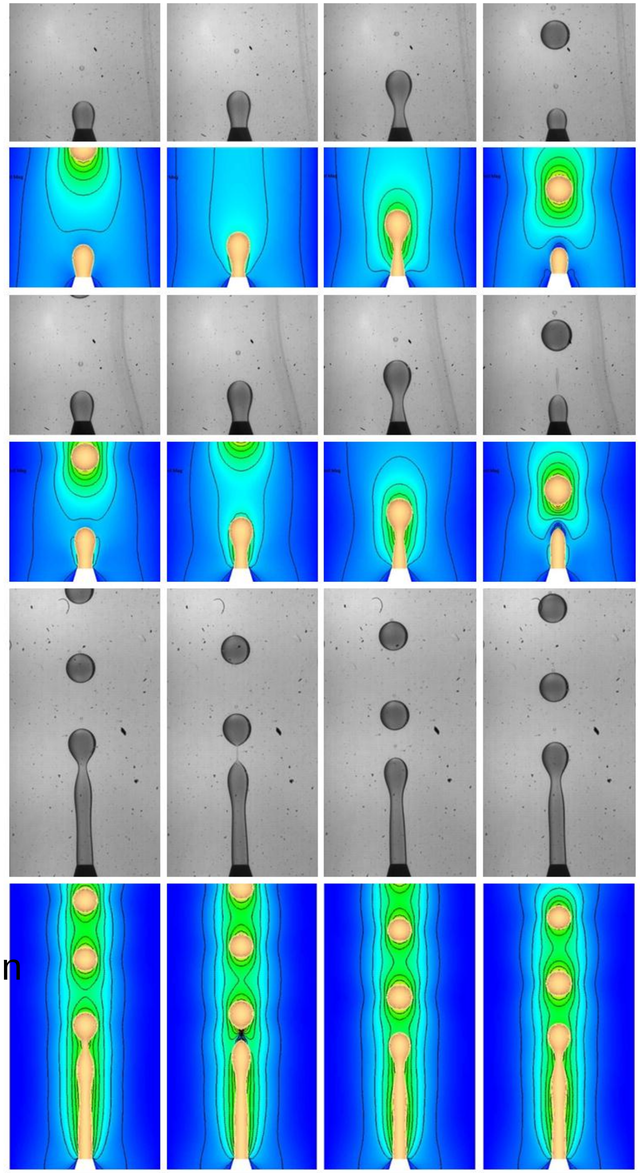


Effects of contact angle?

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

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

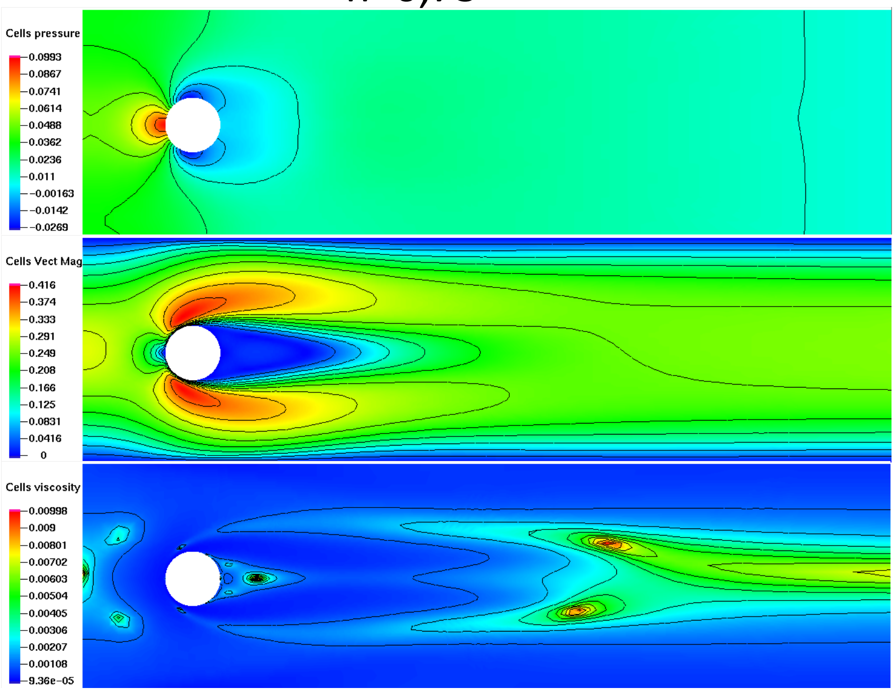


Validation of non-Newtonian rheological models

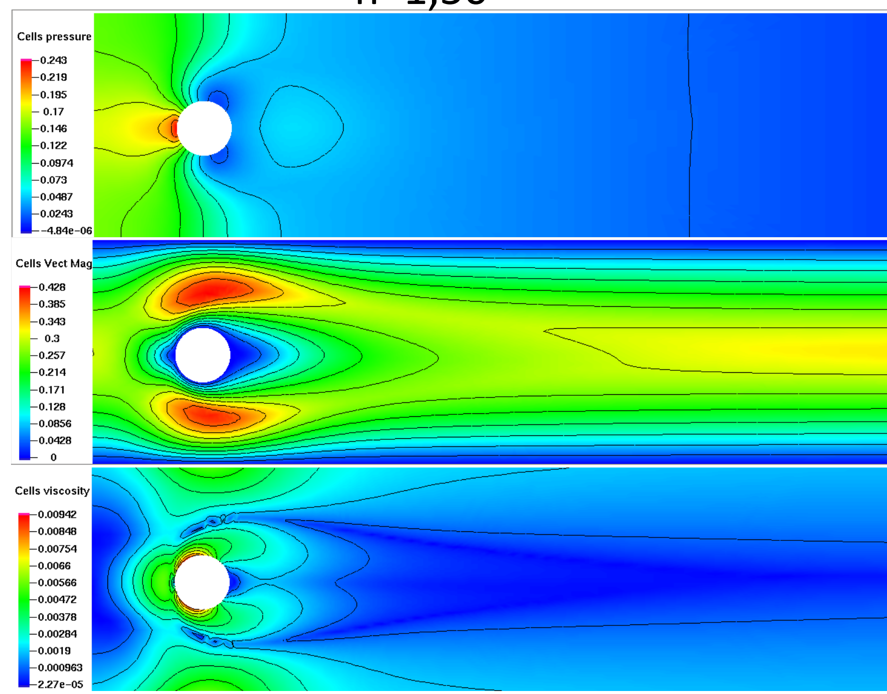
- Power law model
- 2D reference data
- Same discretization
- <u>Same convergence</u>

	Shear thining n=0,75				Shear thickening n=1,50			
	Damanik*		**Our results**		**Damanik***		**Our results**	
level	C_D	C_L	C_D	C_L	C_D	C_L	C_D	C_L
1	3,20082	-0,01261	3,20450	-0,01215	13,6209	0,34250	13,6233	0,34347
2	3,26433	-0,01342	3,26637	-0,01347	13,7380	0,35052	13,7379	0,35037
3	3,27739	-0,01342	3,27755	-0,01343	13,7688	0,34941	13,7688	0,34928

n=0,75



n=1,50



* Damanik, H.; Hron, J.; Ouazzi, A.; Turek, S.: *Monolithic Newton-multigrid solution techniques for incompressible nonlinear flow models*, Ergebnisberichte des Instituts für Angewandte Mathematik Nummer 426, Fakultät für Mathematik, TU Dortmund, 426, 2011

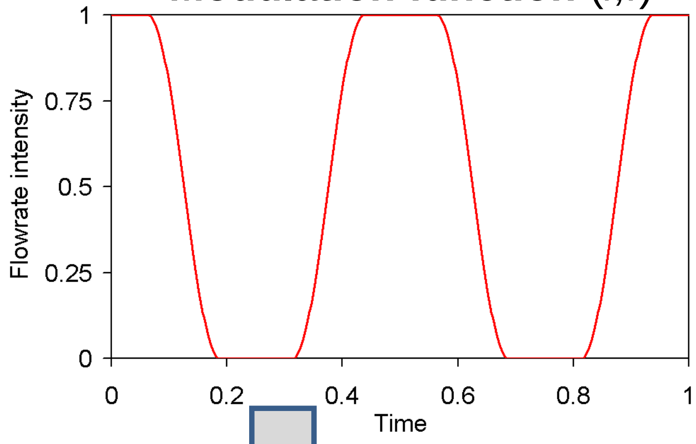
Monodisperse droplet generation

In case of monodisperse droplet generation:

$$\dot{V}_D = f V_{\text{droplet}}$$

1) Droplet generation frequency
2) Regulation frequency

Modulation function (f,I)



Influencable variables

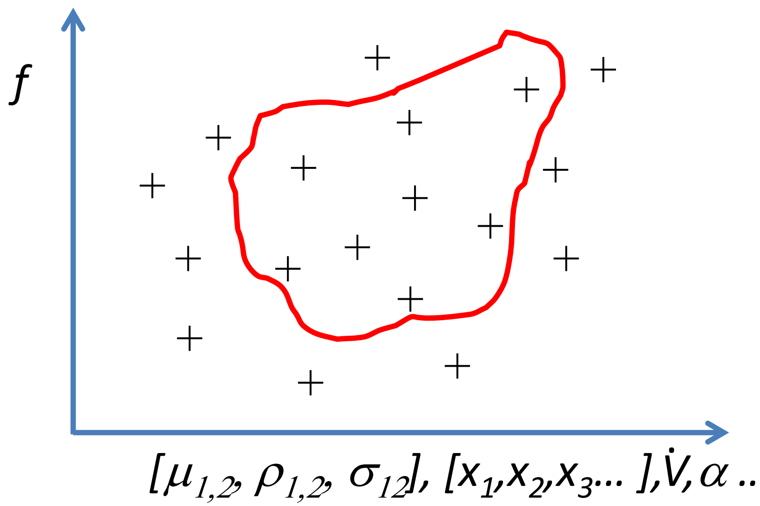
1) Parameters of the process:

- Flowrates
- Modulation frequency
- Modulation amplitude

2) Geometrical changes:

- Capillary size
- Contraction angle
- Contraction ratio

Multidimensional process diagrams



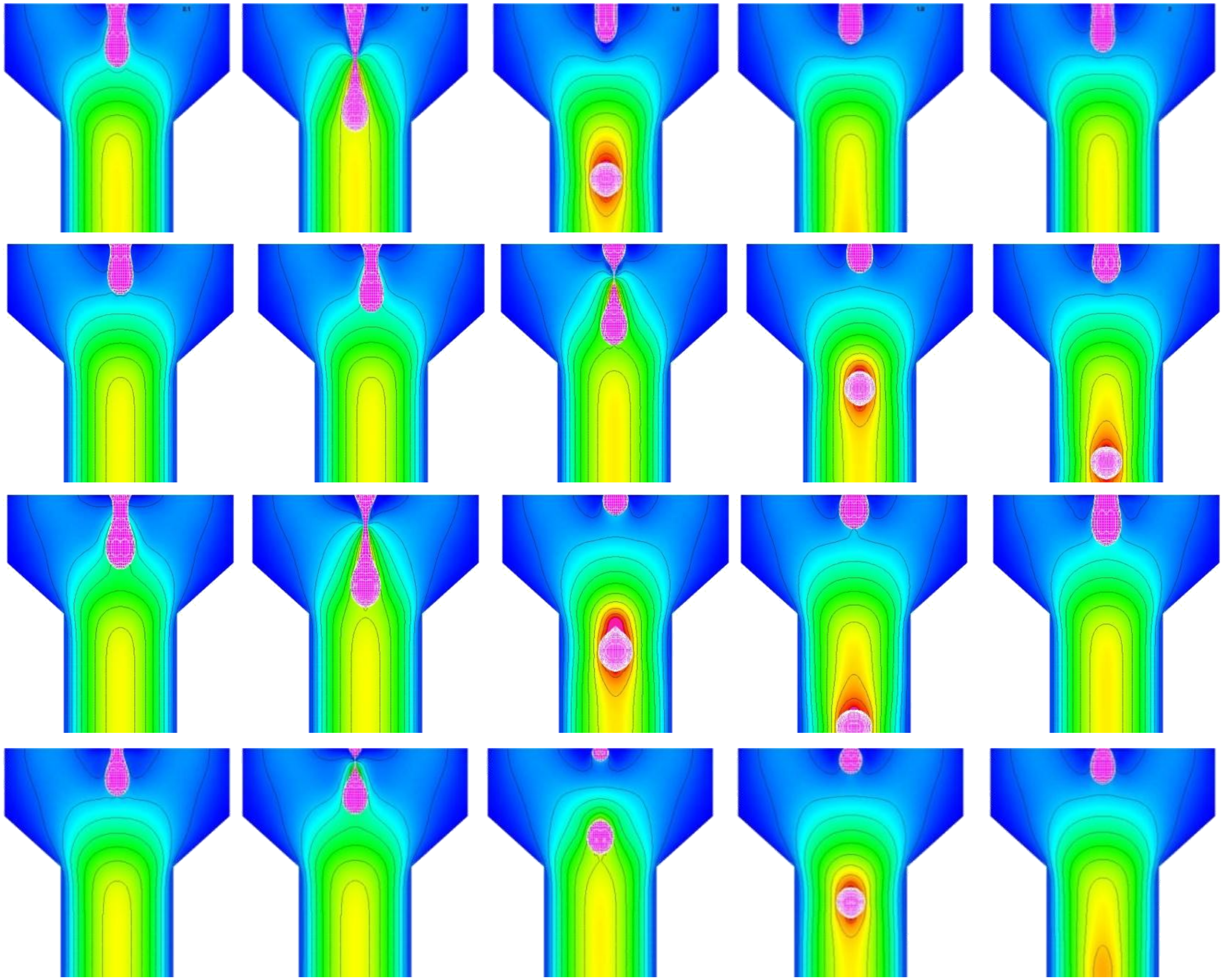
Monodisperse droplet generation in nozzles

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

Conclusions and future tasks

- CFD solver improvement:
  - Non-Newtonian rheological model (Power law) ✓
  - More realistic ratios of physical properties (Validation for Rising Bubble) ✓
  - Implementation of a contact angle model
  - Adaptivity (grid deformation, hanging nodes) ✓
  - HPC (GPU) parallelization

- Application of the developed CFD tool:
  - Testing in wider range of operation conditions ✓
  - Modulation – estimation of ranges for generation of monodisperse droplets ✓
  - Preliminary simulations for non-Newtonian fluids

Validated prediction tool for tailor-made droplet generation
Comparisons, validation, benchmarking

Thank You for Your attention!