Numerische Simulation zur Herrstellung monodisperser Tropfen in pneumatischen Ziehdüsen

DFG – SPP 1423 „Prozess-Spray“

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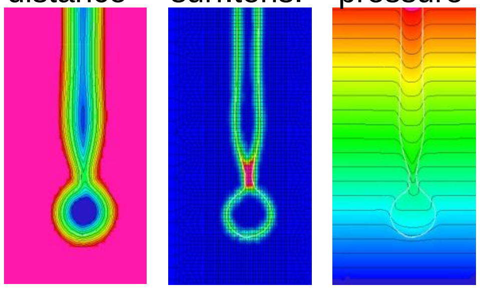
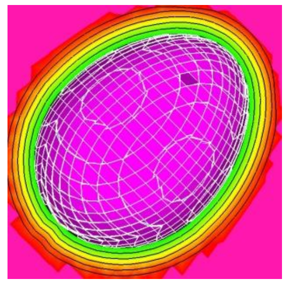
http://www.mathematik.tu-dortmund.de/LS3

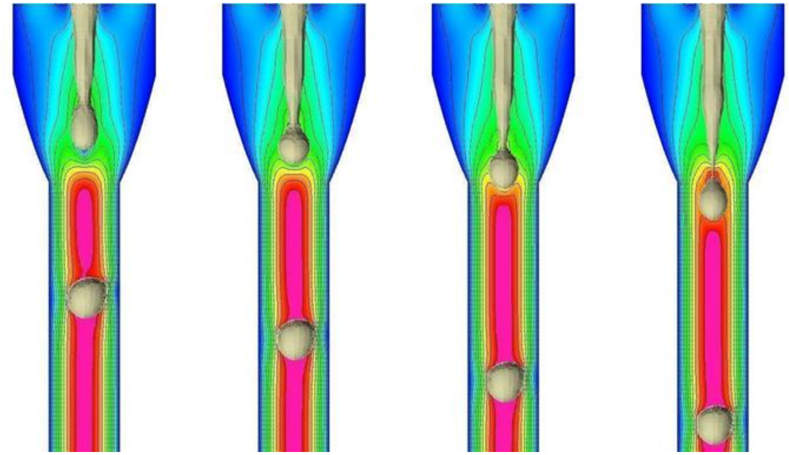
Goals of the first period

1) **Implementation** of a high order mass conservative ALE-based Level Set code

distance surf.tens. pressure

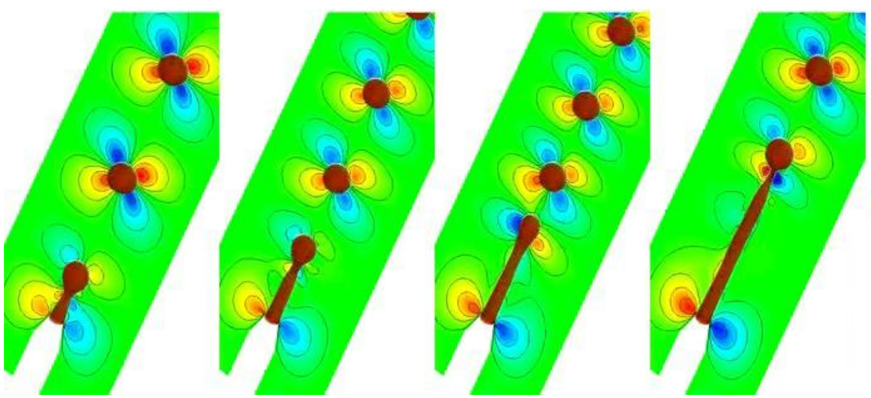




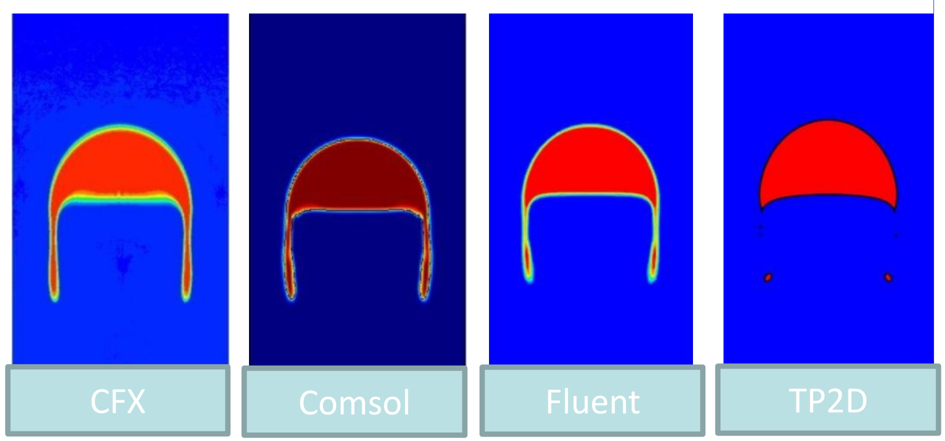


CSF – surface tension treatment PDE-based reinitialisation

2) **Numerical simulation** of droplet generation in dripping and jetting regimes

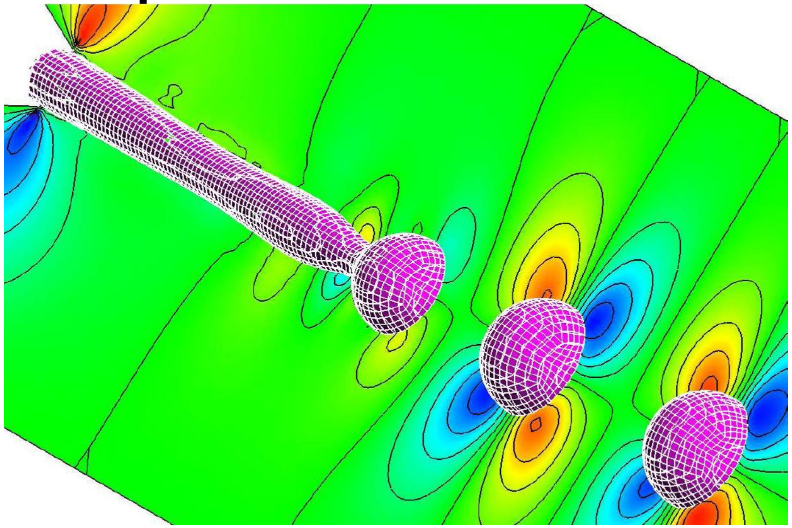


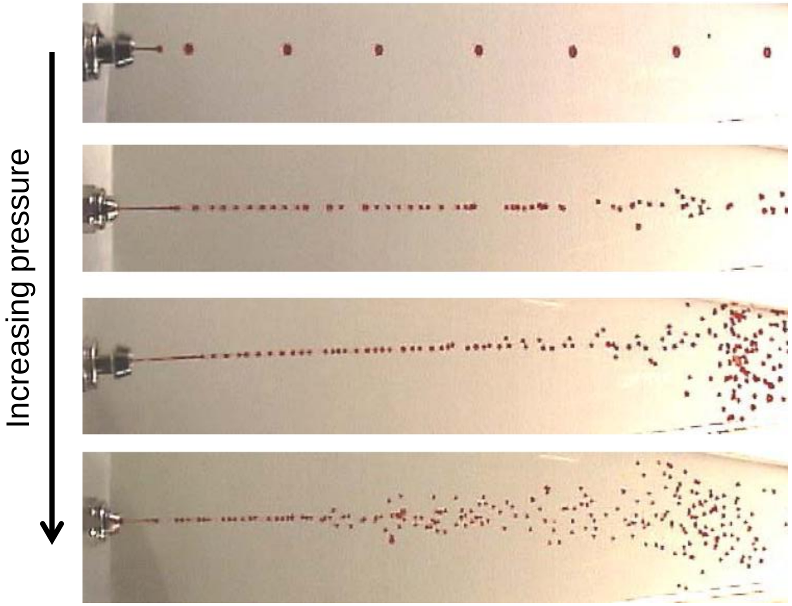
3) **Systematic validation** and benchmarking (CFX, Comsol, FLUENT, OpenFOAM)



Goals of the second period

1) **Jetting mode simulations.**
- Extraction of operation envelopes

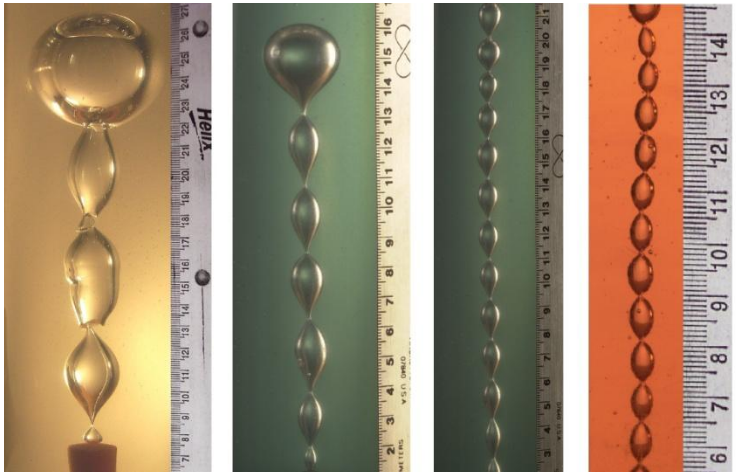




2005 NOVA Chemicals Corporation

2) **Modulation analysis.**
- Multi-dimensional process diagrams

3) **Non-Newtonian fluids.**
- Dripping mode validation
- Jetting simulations
- Multi-dimensional process diagrams



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

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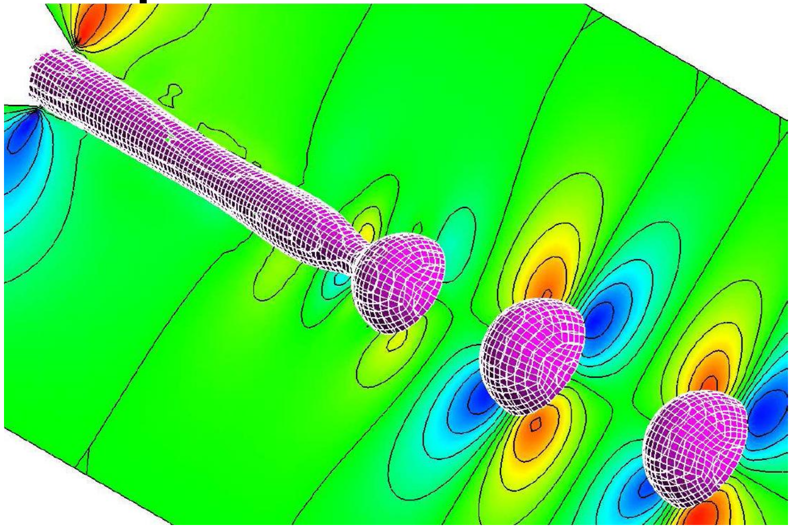
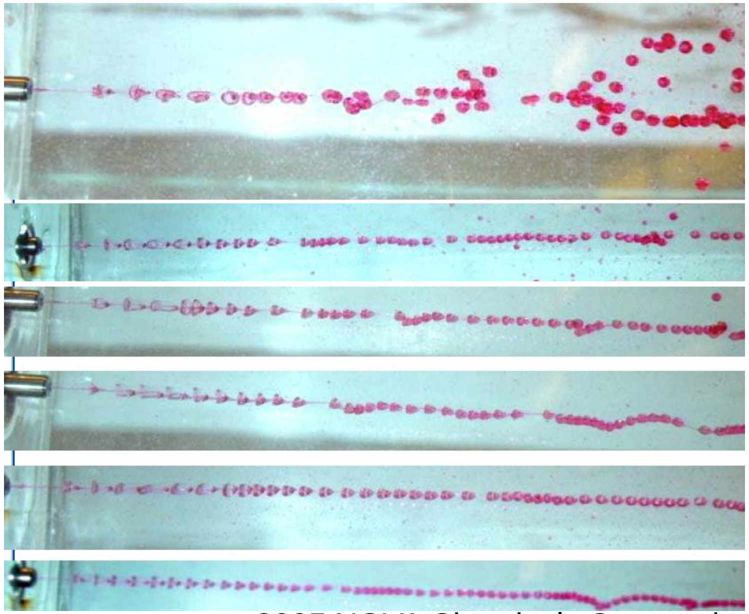
1) **Jetting mode simulations.**
- Extraction of operation envelopes



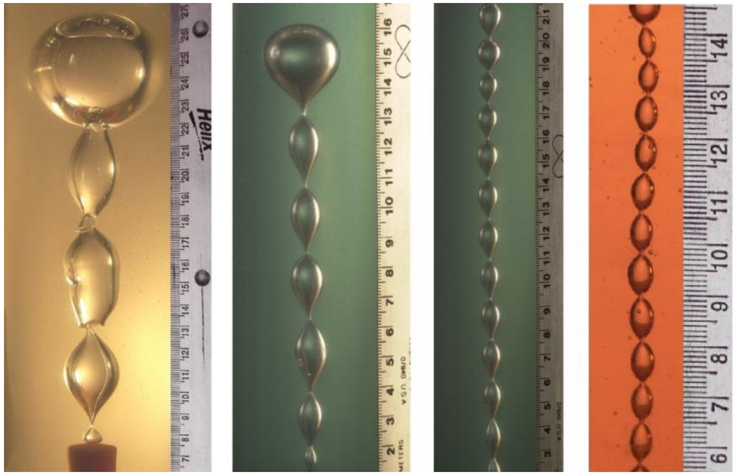
2) **Modulation analysis.**
- Multi-dimensional process diagrams

Increasing pulsation frequancy



2005 NOVA Chemicals Corporation

3) **Non-Newtonian fluids.**
- Dripping mode validation
- Jetting simulations
- Multi-dimensional process diagrams



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

Validation of the dripping mode

Validation parameters:

- frequency of droplet generation
- droplet size
- stream length

Continuous phase:

Glucose-Water mixture

$\mu_D = 500\, mPa\, s$

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

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

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

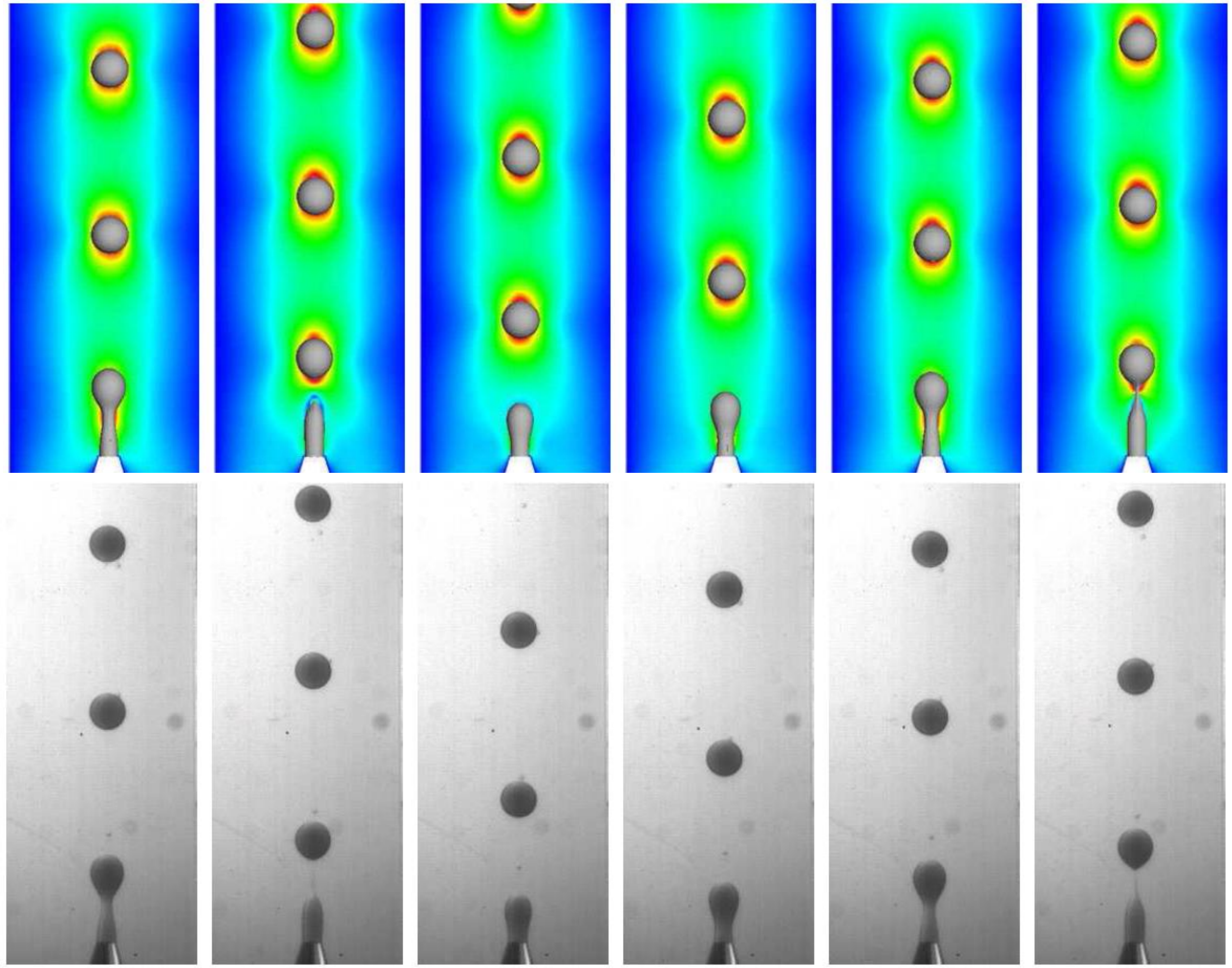
Silicon oil

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

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

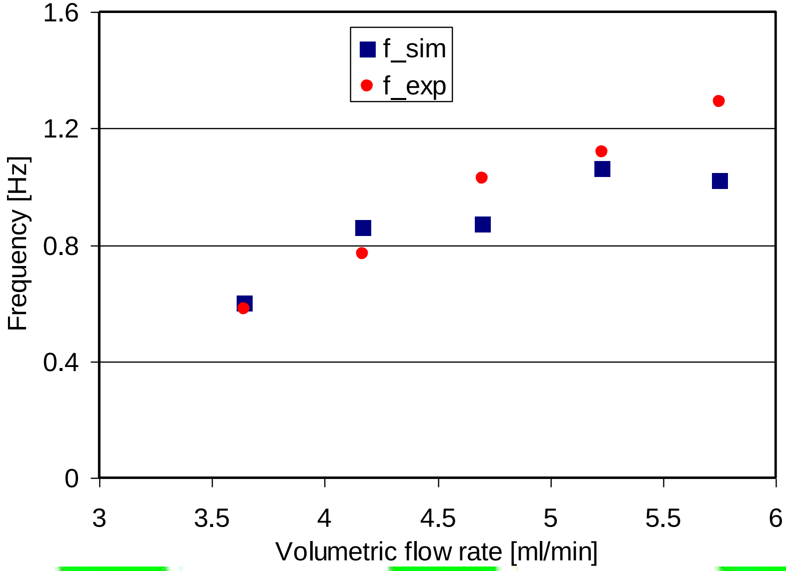
$\dot{V}_C = 99{,}04\, ml min^{-1}$

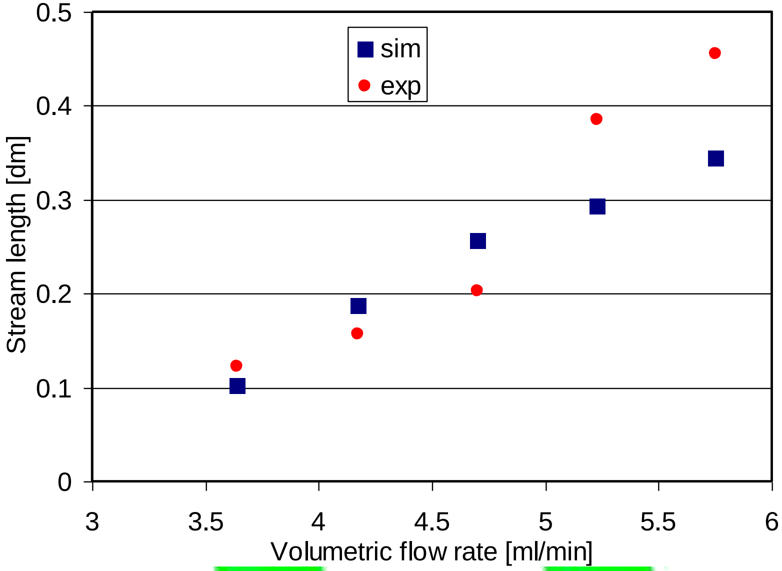
Dispersed phase:

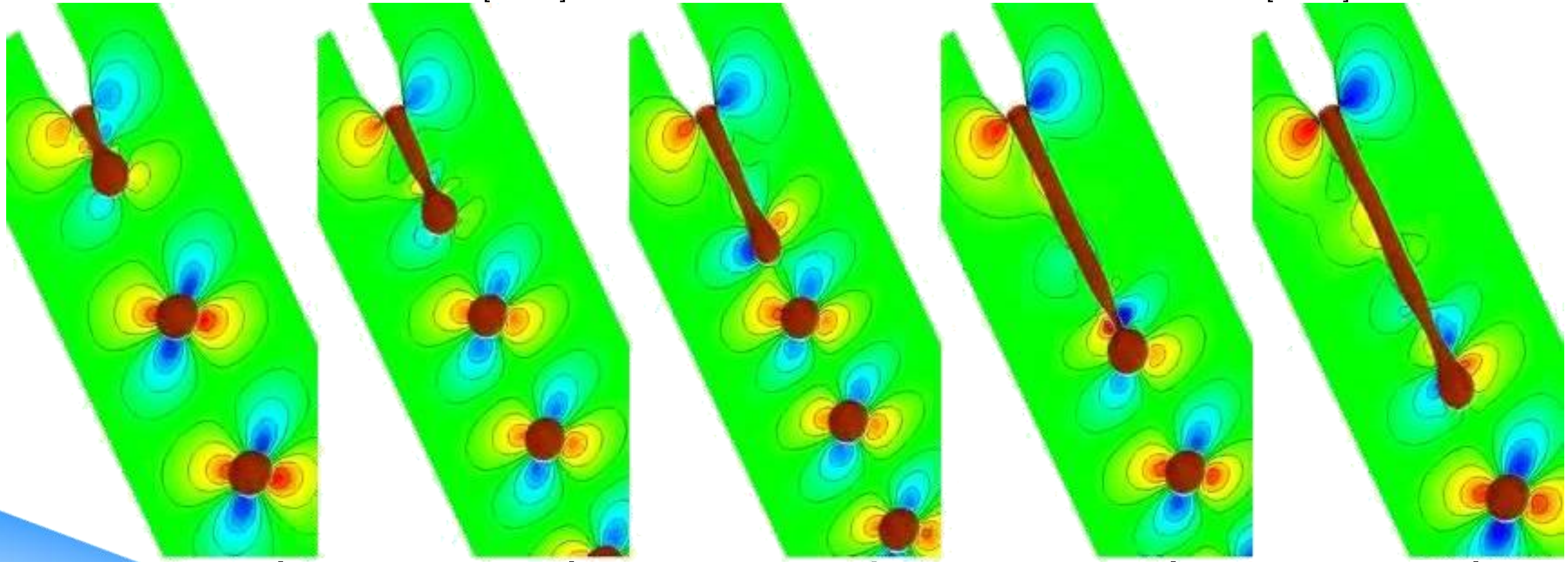


Experimental Set-up with **AG Walzel (BCI/Dortmund)**

Evaluation of the jetting mode





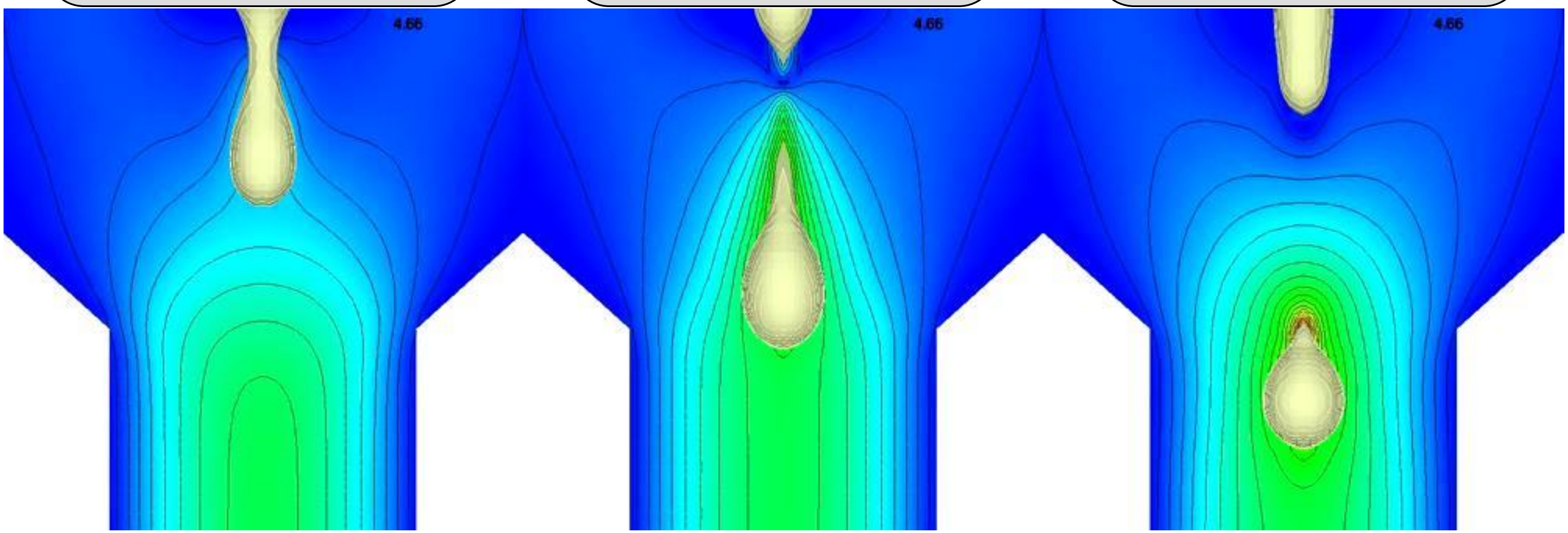


3,64 ml/min 4,17 ml/min 4,70 ml/min 5,23 ml/min 5,75 ml/min

Monodisperse droplet generation in nozzles

In case of monodisperse droplets: $\dot{V}_D = f V_{\text{droplet}}$

With regulation	With regulation	No regulation
$\dot{V}_{D,\text{mean}} = \dot{V}_{STD}$	$\dot{V}_{D,\text{mean}} = 1.5\dot{V}_{STD}$	$\dot{V}_D = \dot{V}_{STD}$



$d_{\text{drop}} = 5.0\,mm$ $d_{\text{drop}} = 5.7\,mm$ $d_{\text{drop}} = 5.2\,mm$

Regulation ranges?
Flow rate ranges?

→ Resulting droplet ranges?

Monodisperse droplet generation in nozzles

In case of monodisperse droplets: $\dot{V}_D = f V_{\text{droplet}}$

Small capillary

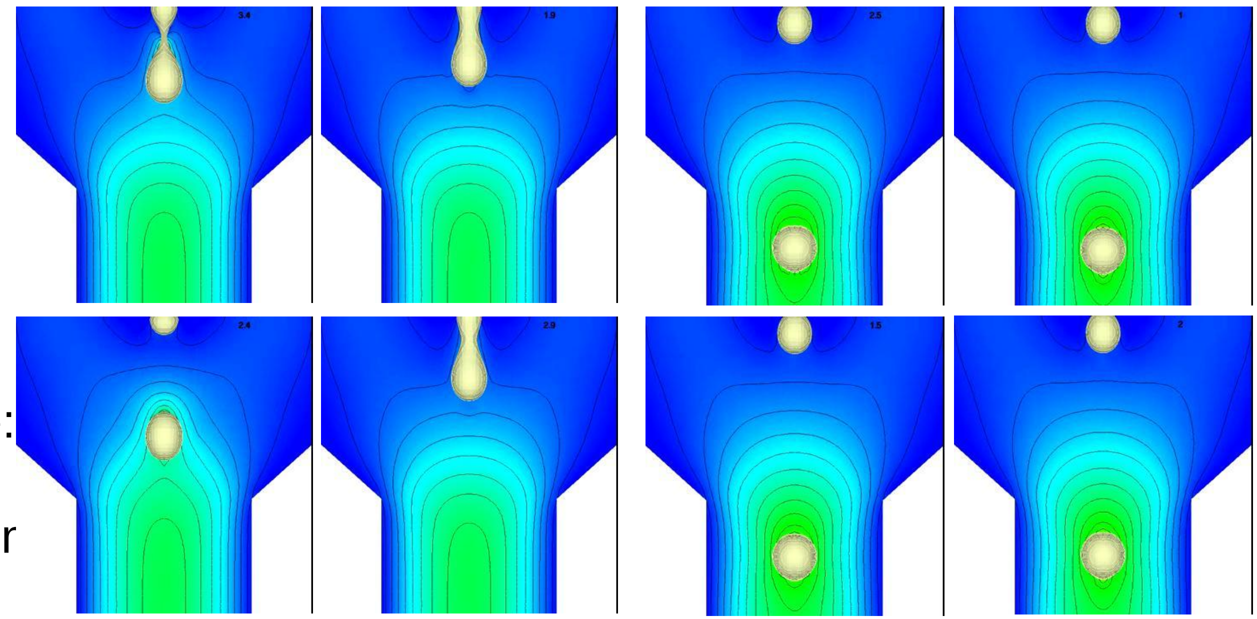
$$\dot{V}_{D,\text{mean}} = 0.75 \dot{V}_{STD}$$

Smaller capillary

$$\dot{V}_{D,\text{mean}} = 0.75 \dot{V}_{STD}$$

Geometrical changes:

- Capillary size
- Contraction angle
- Contraction ratio



Resulting operation envelope:

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

Not monodisperse

Regulation ranges?
Flow rate ranges?

→ Resulting droplet ranges?

Future tasks

Development

- CFD solver improvement w.r.t.:
  - More realistic physical properties
  - Adaptivity
  - HPC (GPU) parallelization
- Non-Newtonian fluids

Process engineering

- Jetting simulations
- Multidimensional process diagrams
- „Rules“ towards optimization
- Droplet-droplet interactions

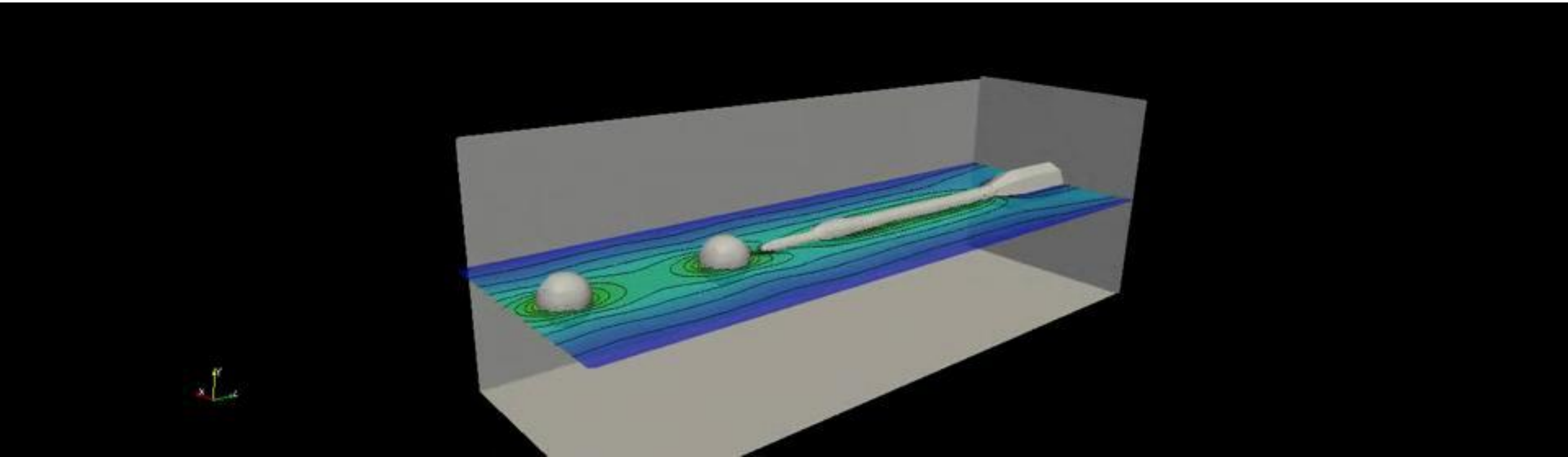
↓

Validated prediction tool for tailor-made droplet generation

Comparisons, validation, benchmarking

Relevant literature:

1) G. Brenn, H. Helpiö, F. Durst: *A New Apparatus for the Production of Monodisperse Sprays at High Flowrates*. 1997, Chem. Eng. Sci. **52**(2), pp. 237—244.
2) M. Orme, Q. Liu, J. Fischer: *Mono-disperse Aluminum Droplet Generation and Deposition for Net-Form Manufacturing of Structural Components*, Eighth International Conference on Liquid Atomization and Spray Systems, Pasadena, CA, USA, July 2000.
3) S.P. Lin, R. D. Reitz: *Drop and Spray Formation from a Liquid Jet*. 1998, Annu. Rev. Fluid Mech. (**30**), pp. 85 — 105.
4) K. Schaake, A. Rudert, R. Schwarze , *Numerical simulation of a modulated axisymmetric liquid ethanol jet injected into air*, 2010, Int. J. of Multif. Flow. (submitted)
5) K.C. Bleijenberg, G. Petela: *A Novel Suspension Polymerization Process Without Mechanical Agitation Yielding Mono-sized Beads*. 2005, NOVA Chemicals.
6) R. P. Chhabra, J. F. Richardson: *Non-Newtonian Flow and Applied Rheology*. 2008
7) S. Turek, O. Mierka, Hysing, S.; Kuzmin, D.: *A high order 3D FEM-Level Set approach for multiphase flow with application to monodisperse droplet generation*, IJNMF, submitted, 2010
8) O. Mierka; S. Turek.: Numerical simulation of monodisperse droplet generation in nozzles, Academic Press, Proceedings of SPRAY 2010 9. Workshop über Sprays, 2010



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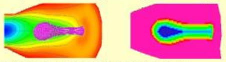
DFG-SPP 1423 „Prozess-Spray“

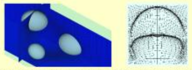
State of the Project

Our FeatFlow based simulation tool:

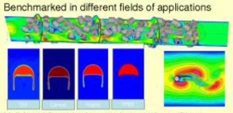
- **High order** (in space and time) **FEM code**
  Q2/P1 FEM in space and Crank Nicholson in time
- Robust parallel multigrid solvers
- Parallel and hardware oriented (GPUs)
- Two phase module supported by *Level Set* approach



- Enhanced by grid deformation techniques



- Benchmarked in different fields of applications



- Validated for dripping mode two phase flows
  Preliminary tests for droplet size oriented modulation
- Preliminary tests for jetting mode
- Implicit treatment of surface tension

Goals & Deliverables

1) Switching the already validated multiphase CFD tool to jetting regime:
   → comparison with experimentally available results
   → identification of the "Rayleigh" and "first wind-induced" subregimes in terms of non-dimensional numbers
   → gathering data via simulations in the appropriate subregimes

2) Analysis of modulation and imposition of disturbances in the appropriate subregimes:
   → analysis of the possibilities of modulation (where to impose it? manipulation of frequency or amplitude?)
   → comparison with experimentally available results
   → outline the ranges of conditions leading to monodisperse droplet generation

3) Extension to non-Newtonian fluids:
   → Dripping mode validation based on experimental results
   → repetition of points 1) and 2) for different shear dependent models

- **Contribution to the engineering community with an open-source CFD-based prediction tool suitable for tailor-made droplet generation**
- **Contribution to the scientific community with two-phase flow 3D benchmark configurations**
- **Multidimensional process diagrams for the interpretation of rules for accessible monodisperse operation ranges**

Tasks

Solver

- CFD solver improvement w.r.t.:
  - More realistic physical properties
  - Enrichment with Grid Deformation Technique
  - Acceleration by GPU parallelization
- Extension to non-Newtonian fluids

Application

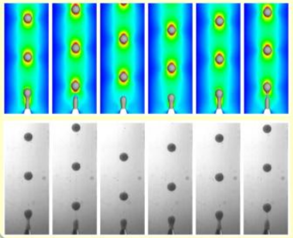
- Validation within the jetting regime
- Process modulation
- Construction of multidimensional process diagrams for the involved parameters
- Investigation of downstream coalescence effects on the dispersity of droplets

Cooperation

- Experimental measurements supported by group and facilities of **AG Walzel**
- Extensive compute power supported by the **Linux Cluster LiDO**
- Simulation cooperation partners: **AG Bothe**, **AG Sommerfeld**, **AG Schwarze**

Validation & Benchmarking

Dripping mode



Continuous phase:
Glucose-Water mixture
$\mu_D = 500\,\mathrm{mPa\,s}$
$\rho_D = 972\,\mathrm{kg\,m^{-3}}$
$\dot{V}_D = 3{,}64\,\mathrm{ml\,min^{-1}}$

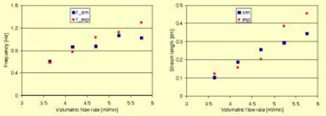
Dispersed phase:
Silicon oil
$\mu_C = 500\,\mathrm{mPa\,s}$
$\rho_C = 1340\,\mathrm{kg\,m^{-3}}$
$\dot{V}_C = 99{,}04\,\mathrm{ml\,min^{-1}}$

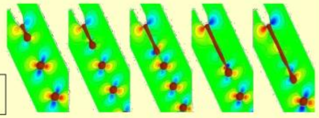
$\sigma_{CD} = 0{,}034\,\mathrm{N\,m^{-1}}$

	Separation frequency [Hz]	Droplet size [dm]	Stream Length [dm]
Exp	0,58	0,062	0,122
Sim	0,60	0,058	0,102

All experimentally measured results are provided by **AG Walzel**

Jetting mode





Recent Modulation Results

In case of monodisperse droplet generation:

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

Influencable variables
On the process level:
- Flowrates
- Modulation frequency
- Modulation amplitude

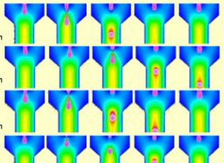
Geometrical changes:
- Capillary size
- Contraction angle
- Contraction ratio

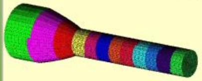
No Regulation
Flowrate: 100%
Capillary: STD
Droplet size: 5.2mm

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

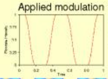
Regulated
Flowrate: 150%
Capillary: STD
Droplet size: 5.7mm

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

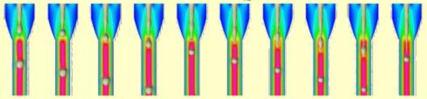




Applied modulation

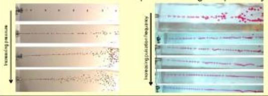


Resulting operation envelope:
- Size: 4.5 mm – 5.7 mm
- Volume: 0.38 cm^3 – 0.77 cm^3



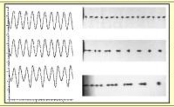
Guidelines, References

→ Nova Chemicals : Mono-dispersion of organic phase by pulse atomization



- Pressure pulsation leads to volumetric flowrate pulsation
- Modulation of frequency and amplitude
- Newtonian and non-Newtonian

→ Orme et al.:
Mono-disperse Aluminum droplet generation and deposition for Net-Form Manufacturing of Structural Components



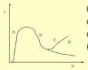
- Amplitude modulation with constant frequency
- Targeted coalescence of generated droplets
- Increases the ranges of achievable droplets

→ Brenn et al.:
A new apparatus for the production of monodisperse sprays at high flowrates

$$d = \left(\frac{3uD^2}{2f}\right)^{\frac{1}{3}}$$

- Introduction of disturbances with certain frequencies *f*
- Validity of regulation in ranges of Re numbers
- 2-4% standard deviation of droplet diameters

→ Lin et al.:
Drop and sray formation from liquid jet



Classification of jets depending on non-dimensional quantities (Re, We, etc.)

→ Chhabra, Non-Newtonian Flow And Applied Rheology