# Numerische Simulation zur Herstellung monodisperser Tropfen in pneumatischen Ziehdüsen

DFG – SPP 1423 „Prozess-Spray“

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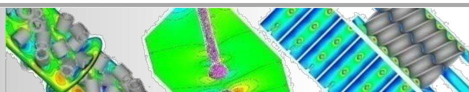
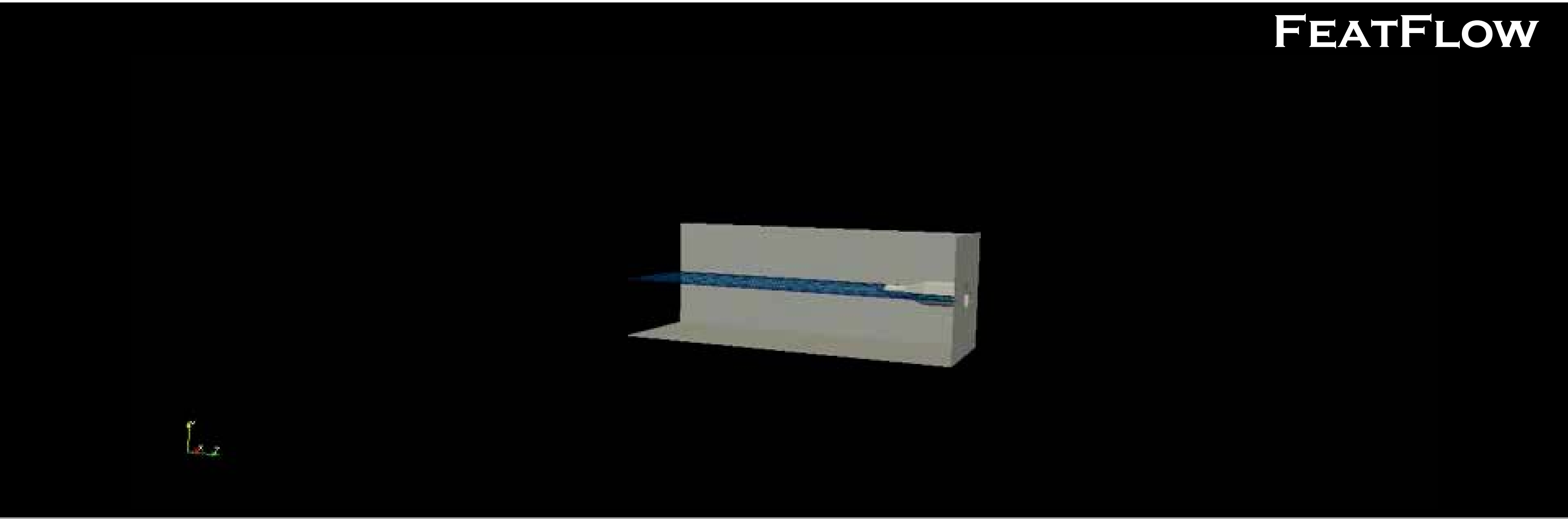
http://www.featflow.de
http://www.mathematik.tu-dortmund.de/LS3



# Main Goals

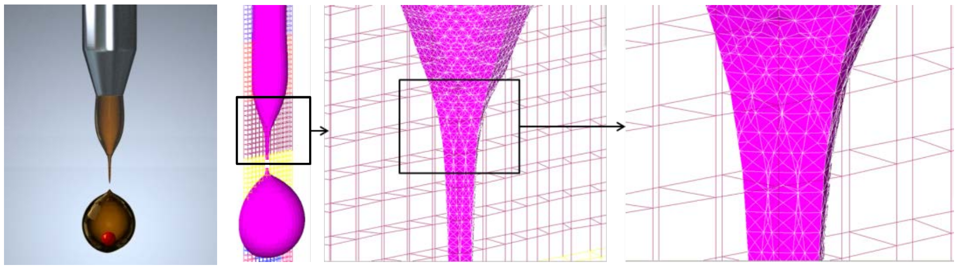
***CFD simulation of monodisperse droplet generation by means of jet break-up***
***→ Geometry, material parameters, rheological properties, modulation***

| 1st period | 2nd period | 3rd period |
|---|---|---|
| - LS-FEM | - mgLS-FEM | - mgLS[(2)]-FBM-FEM |
| • Benchmarking and Validation | • Gas/liquid-like systems | • Gas/liquid/solid systems with Non-Newtonian fluids |
| • Droplet dripping | • Non-Newtonian models | • Multiple Level Set or FBM |
| • Modulation | • Jetting regime | • Modulation |
| | • Wider range of Op. Cond. | |



# The Flow Solver mgLS-FEM

Basic slow solver – **FEATFLOW**
(robust, parallel, efficient)



**Numerical features:**

- Higher order Q2P1 FEM schemes
- FCT & EO FEM stabilization techniques
- Use of unstructured meshes
- Fictitious Boundary (FBM) methods
- Dynamic adaptive grid deformation
- Newton-Multigrid solvers

**Non-newtonian flow module:**

- generalized Newtonian model (Power-law, Carreau, ... etc.)
- viscoelastic model (Giesekus, Oldroyd B, …etc.)

**Multiphase flow module (resolved interfaces):**

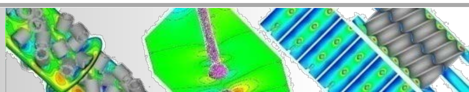
- *l/l* – interface tracking method (levelset)
- *s/l* – interface capturing method (FBM)
- *s/l/l* – combination of *l/l* and *s/l*

**Engineering aspects:**

- Geometrical design
- Modulation strategy
- Optimization

**FEM-based simulation tool for the accurate prediction of „tailor-made“ droplet generation within encapsulation processes**



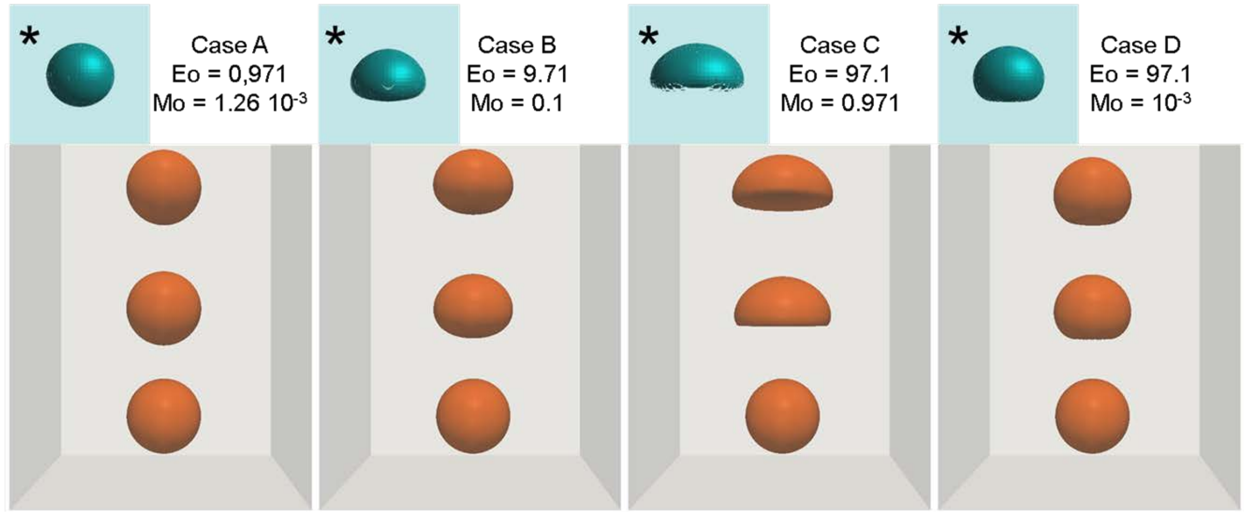


# Validation of the mgLS-FEM Flow Solver

**3D rising Bubble**

References:
- Annaland et al.,
- Clift and Grace

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



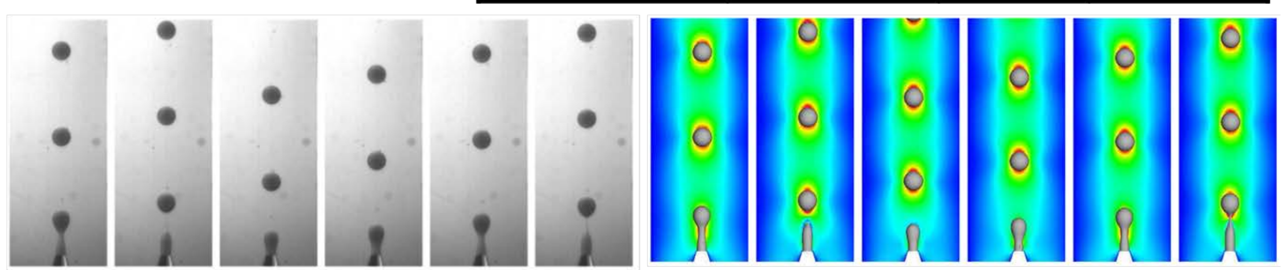

| Case A | Case B | Case C | Case D |
|---|---|---|---|
| $Re_{ExpRef} = 1.7$ | $Re_{ExpRef} = 4.6$ | $Re_{ExpRef} = 20$ | $Re_{ExpRef} = 1.5$ |
| $Re_{SimRef} = 1.6$ | $Re_{SimRef} = 4.3$ | $Re_{SimRef} = 18$ | $Re_{SimRef} = 1.7$ |
| $Re_{Sim} = 1.57$ | $Re_{Sim} = 4.39$ | $Re_{Sim} = 17.2$ | $Re_{Sim} = 1.58$ |

**3D droplet dripping**

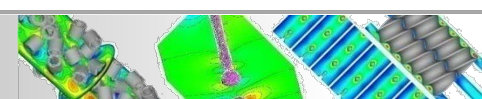
References:
- BCI Dortmund (AG Walzel)
- iRMB Braunschweig

Water glucose mixture
&
Silicone oil

| Group | Separation frequency [Hz] | Droplet size [dm] | Stream Length [dm] |
|---|---|---|---|
| BCI Dortmund | 0,58 | 0,062 | 0,122 |
| iRMB Braunschweig | 0,37 | 0,068 | 0,113 |
| AM&N Dortmund | 0,60 | 0,058 | 0,102 |







# Tailored Monodisperse Droplets via Modulation

**In case of monodisperse droplet generation:**

$$\dot{V}_D = f\, V_{drop}$$

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

**Influenceable variables**

On the level of the process:

- Flow rates
- Modulation frequency
- Modulation amplitude

Geometrical changes:

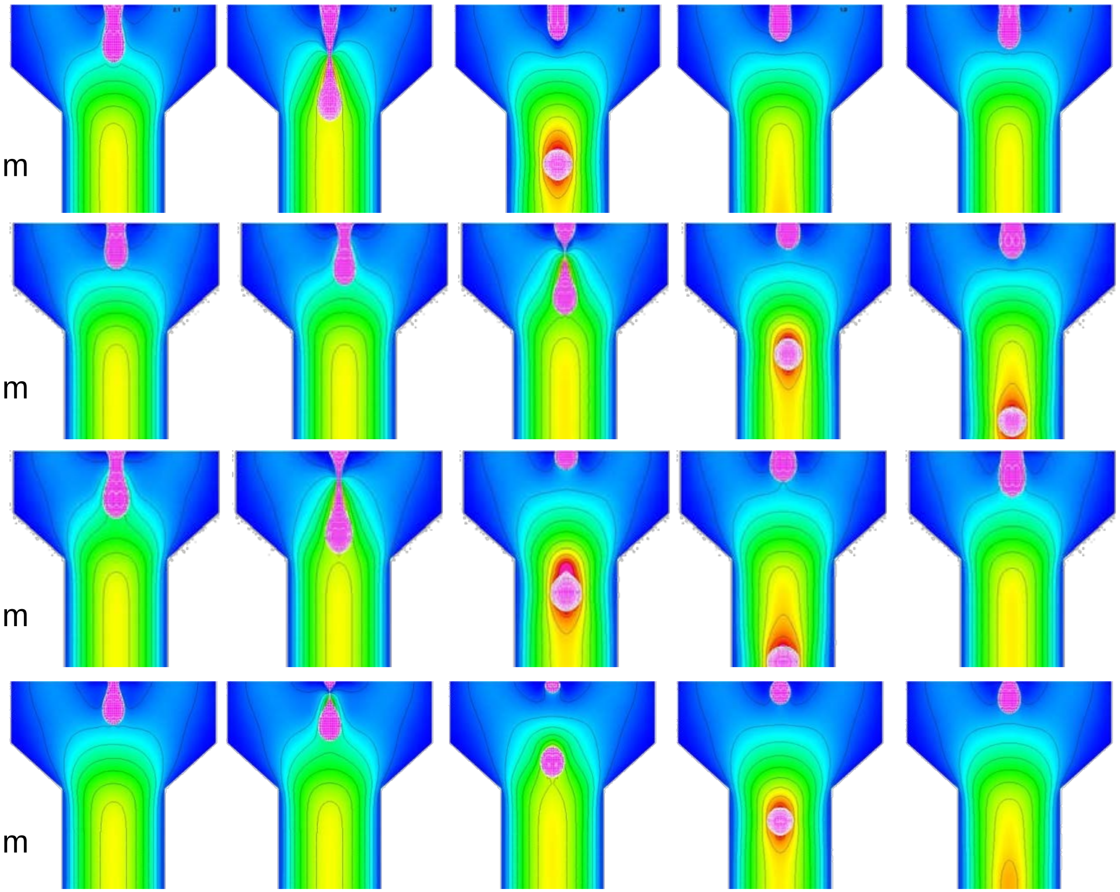
- Capillary size
- Contraction angle
- Contraction ratio

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

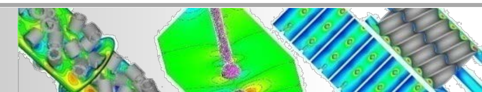


G. Brenn, T. Helpiö and F. Durst, A new apparatus for the production of monodisperse sprays at high flow rates,  Chem. Eng. Sci. (1997) **52**, 237-244.

**Resulting operation envelope:**

- **Size: 4.5 mm – 5.7 mm**
- **Volume: 0.38 cm³ – 0.77 cm³**



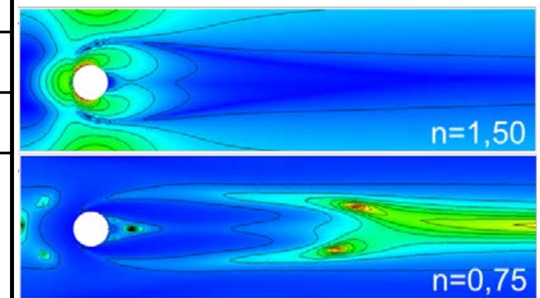


# Non-Newtonian Flow Module - Validation

## Single phase validation on 2D benchmark “flow around a cylinder”

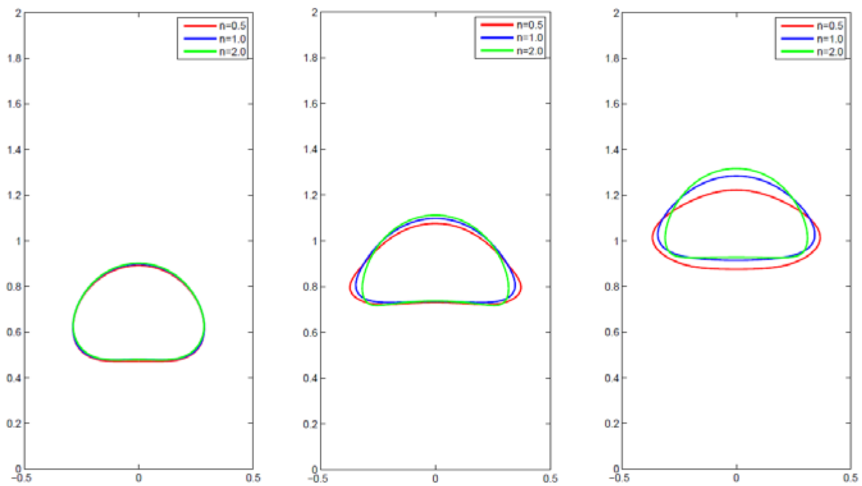
Reference: Damanik et al.

| | Shear thinning 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 |



Viscosity distribution

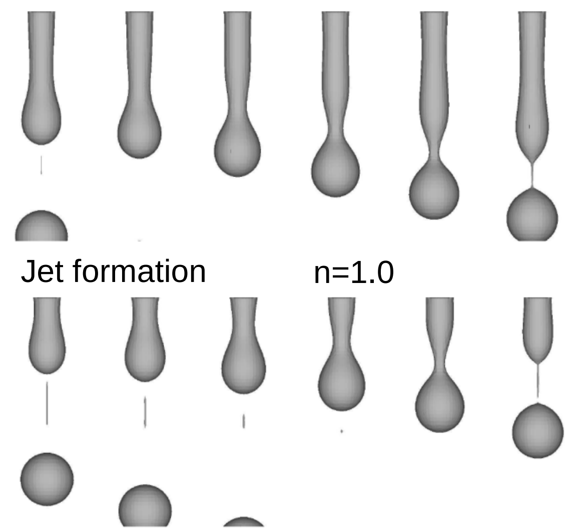
## Pseudo 2D rising bubble in Power-Law fluids

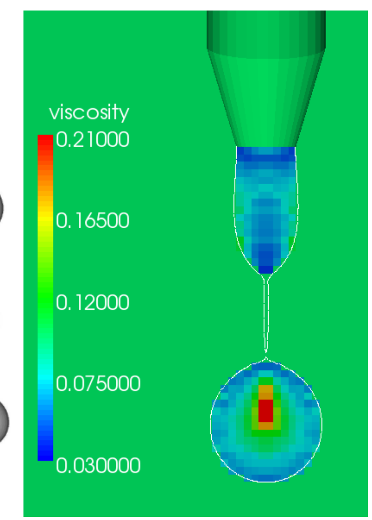


Mesh converged bubble shapes for n = 0.5, 1.0, 2.0

To do: L. Zhanga et al. Numerical simulation of a bubble rising in shear-thinning fluids, *J. Non-Newt. Fl. Mech.*

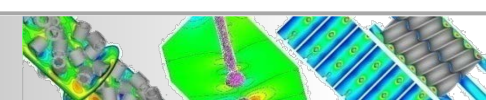
## Droplet generation for Power-Law fluids



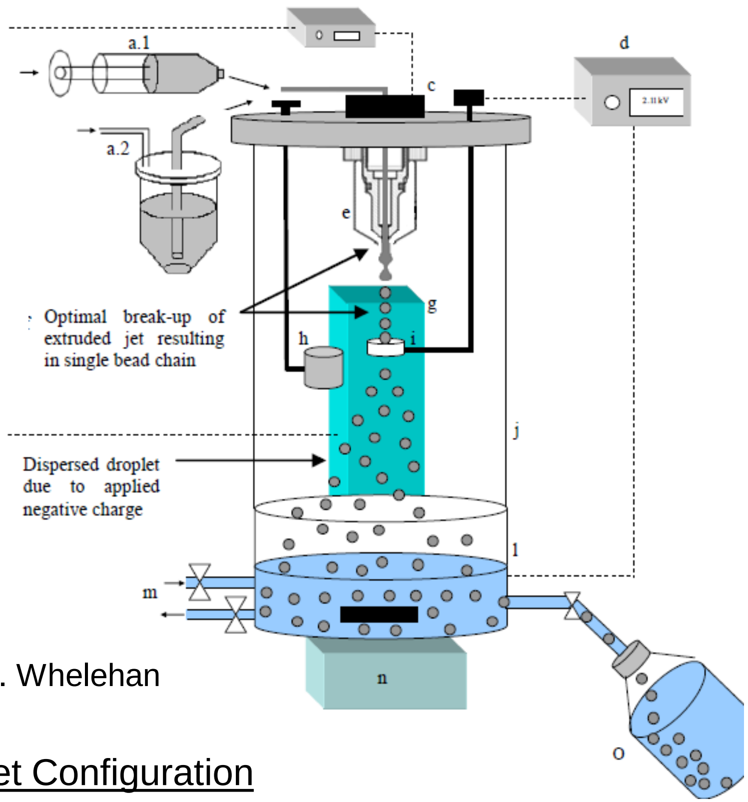
Instanteous viscosity distribution for n=0.5





# Next Goals: Simulation of Encapsulation Processes

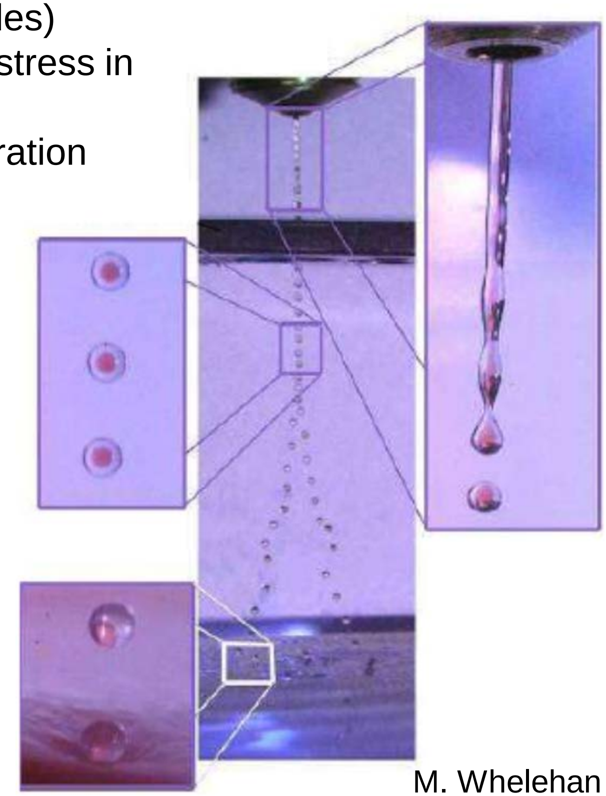
- Numerical simulation of *micro-fluidic drug encapsulation (“monodisperse compound droplets”)*
- Polymeric “bio-degradable” outer fluid with generalized Newtonian behaviour
- Optimization w.r.t. boundary conditions, flow rates, droplet size, geometry




M. Whelehan

<u>In Pharmaceutics</u>

- Controlled drug release
- Protection of chemically active ingredients (from both sides)
- Protection against shear stress in stirred reactors
- Protection against evaporation
- Taste or odor masking



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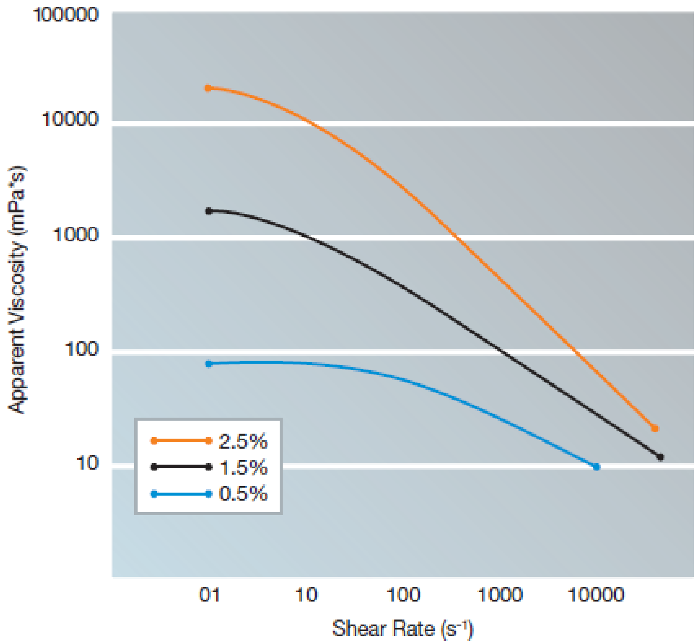
<u>Jet Configuration</u>

- Core material is defined as the specific material that requires to be coated (liquid, emulsion, colloid or solid)
- Shell material is present to protect and stabilize the core (Alginate, Chitosan, Gelatin, Pectin, Waxes, Starch)

# Encapsulation

| | Tasks related to code development | Tasks related to application |
|---|---|---|
| mgLS[(2)]-FBM-FEM flow module | • Multiple Level Set fields for simulation of liquid core encapsulation - l/l/g<br>• Fictitious boundary method for particle encapsulation - s/l/g | • Validation via experimental results<br>• Modulation for monodisperse compound drops |

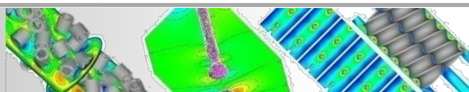

Aqueous solutions of alginates have shear-thinning characteristics




**Work program:**

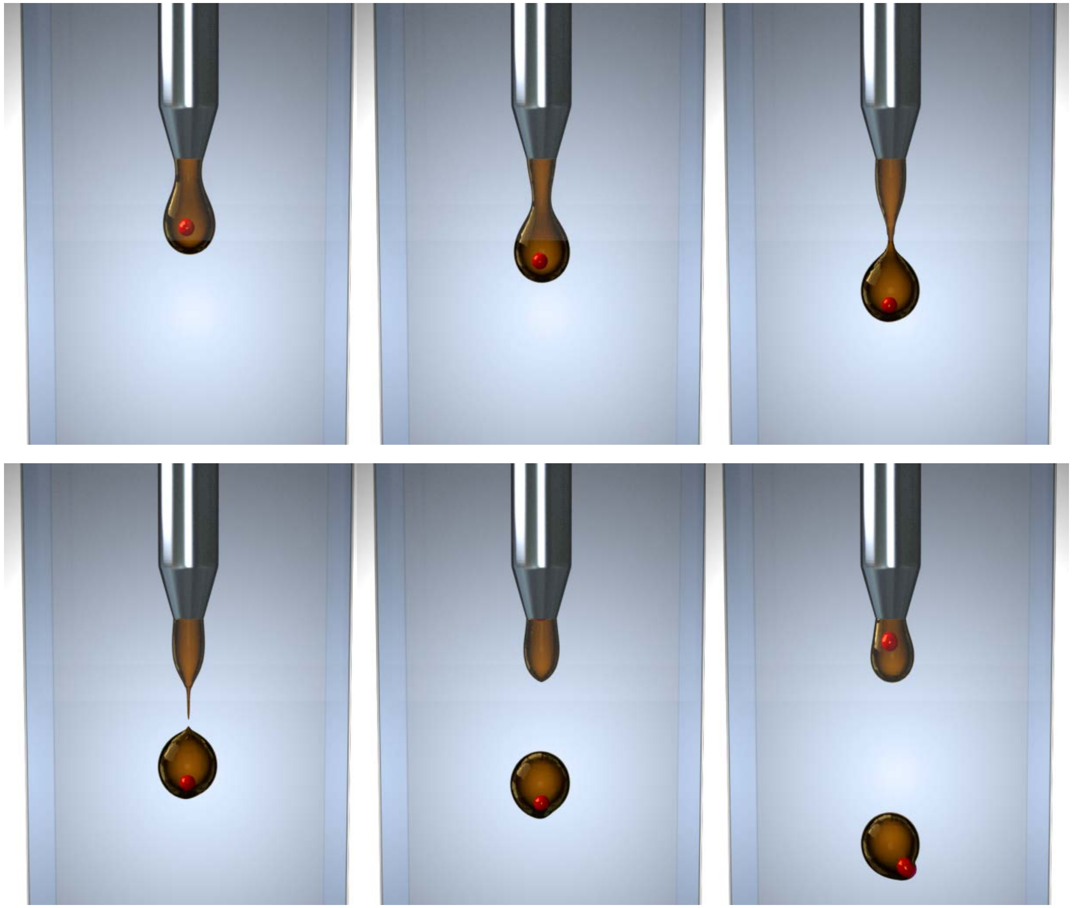
- Validation of the non-Newtonian multiphase flow solver (on 3D rising bubbles)
- Validation of droplet generation with pure (shear thinning) alginate solutions
- Extension of the flow solver with the corresponding three phase modules
- Validation of droplet generation within encapsulation process
- Investigation of operation envelopes for monodisperse compound drop generation





# Preliminary Encapsulation Results

Preliminary simulation results of a periodic particle encapsulation process.
The particle sampling frequency is identical with the droplet dripping frequency.



# Literature based Validation

Drop formation by means of Non-Newtonian (shear thinning) fluids


- M. R. Davidson, J. J. Cooper-White, Pendant drop formation of shear-thinning and yield stress fluids, App. Math.l Mod. **30** (2006) 1392–1405.
- Ö. E. Yıldırım, O. A. Basaran, Dynamics of formation and dripping of drops of deformation-rate-thinning and -thickening liquids from capillary tubes, J. Non-Newt. Fl. Mech. **136** (2006) 17–37.
- R. Suryo, O. A. Basaran, Local dynamics during pinch-off of liquid threads of power law fluids: Scaling analysis and self-similarity, J. Non-Newt. Fl. Mech. **138** (2006) 134–160.


## Thank You for Your attention

Literature on encapsulation:


- M. Whelehan, Liquid-core microcapsules: A mechanism for the recovery and purification of selected molecules in different environments, PhD Thesis, 2010, Dublin.
- S.-L. Chiu and T.-H. Lin, Breakup of compound liquid jets under periodic excitation at small core-to-shell mass ratios, J. Chin. Inst. Eng. **31**, 2008.
- A.F. Berger, Herstellung monodisperser Partikel aus einer wässerigen Lösung mittels Fluidprillen/ Gefriertrocknen oder chemischer Reaktion, PhD Thesis, Zurich, 2001.
- P. D. Gaudio, P. Russo, M. R. Lauro, P. Colombo and R. P. Aquino, Encapsulation of Ketoprofen and Ketoprofen Lysinate by Prilling for Controlled Drug Release, AAPS Pharm-SciTech, **10**, 2009..