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

<table>
<thead>
<tr>
<th>1st period</th>
<th>2nd period</th>
<th>3rd period</th>
</tr>
</thead>
<tbody>
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<td>LS-FEM</td>
<td>mgLS-FEM</td>
<td>mgLS((2))-FBM-FEM</td>
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<td>Benchmarking and Validation</td>
<td>Gas/liquid-like systems</td>
<td>Gas/liquid/solid systems with Non-Newtonian fluids</td>
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<td>Droplet dripping</td>
<td>Non-Newtonian models</td>
<td>Multiple Level Set or FBM</td>
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<tr>
<td>Modulation</td>
<td>Jetting regime</td>
<td>Modulation</td>
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</tbody>
</table>
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

3D droplet dripping

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

Water glucose mixture & Silicone oil

<table>
<thead>
<tr>
<th>Group</th>
<th>Separation frequency [Hz]</th>
<th>Droplet size [dm]</th>
<th>Stream Length [dm]</th>
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</thead>
<tbody>
<tr>
<td>BCI Dortmund</td>
<td>0.58</td>
<td>0.062</td>
<td>0.122</td>
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<tr>
<td>iRMB Braunschweig</td>
<td>0.37</td>
<td>0.068</td>
<td>0.113</td>
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<tr>
<td>AM&amp;N Dortmund</td>
<td>0.60</td>
<td>0.058</td>
<td>0.102</td>
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</tbody>
</table>
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


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”

<table>
<thead>
<tr>
<th>Level</th>
<th>Shear thinning n=0.75</th>
<th>Shear thickening n=1.50</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>Damanik*</td>
<td>Our results</td>
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<tr>
<td>1</td>
<td>C_D</td>
<td>C_L</td>
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<tr>
<td>3,20082</td>
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<tr>
<td>3</td>
<td>3,27739</td>
<td>-0.01342</td>
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</tbody>
</table>

Reference: Damanik et al.

Viscosity distribution

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

In Pharmaceutics
- 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

Jet Configuration
- 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

- Multiple Level Set fields for simulation of liquid core encapsulation
- Fictitious boundary method for particle encapsulation

Tasks related to application

- Validation via experimental results
- Modulation for monodisperse compound drops

Aqueous solutions of alginates have shear-thinning characteristics

mgLS\textsuperscript{(2)}-FBM-FEM flow module

**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 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

Thank You for Your attention

Literature on encapsulation: