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 objectives of the project

• Development of a fast and accurate CFD-based simulation tool suitable for non-Newtonian multiphase problems. Extension of the standard FeatFlow solver with additional packages
  - Level Set Method for interface capturing
  - Generalized Newtonian rheological models
  - ALE Method with dynamic mesh deformation

• Multistage validation of the simulation tool w.r.t experimental measurements or computational benchmarks

• Simulation of encapsulation (3-phase) processes:
  - under modulated conditions
  - materials obeying shear thinning rheological models
Continuity of development within SPP 1423

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

→ Geometry, material parameters, rheological properties, modulation

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**Modulation example**

Newtonian jetting example

Non-Newtonian two phase flow

Encapsulation process
Encapsulation processes

- Numerical simulation of *micro-fluidic drug encapsulation* ("monodisperse compound droplets")
- "Bio-degradable" outer liquid with *generalized Newtonian* behaviour
- Optimization w.r.t. boundary conditions, flow rates, droplet size, geometry, modulation

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)

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
Numerical challenges of the encapsulation process

Individual difficulties:
- Moving interfaces (g-l-l)
- Large ratios of physical properties
- Surface tension effects
- Non-Newtonian fluids

Numerical techniques:
- Level Set for tracking of multiple interfaces
- Mesh deformation with ALE for optimal resolution of the interface
- Complex rheological fluid properties:
  - Generalized Newtonian models (shear thinning)

Air (vacuum) as ambient material

Excitation of the nozzle with the aim of modulation

Coaxial arrangement of the nozzles

Inner core material (drugs, special agents)

Outer carrier shell (alginate)

Operation envelopes for modulation

Shear dependent viscosity of alginate

Otto Mierka
Modular structure of mgLS\(^{(2)}\)-FEM

**Numerical features of FEATFLOW:**
- Higher order Q2P1 FEM schemes
- FCT & EO FEM stabilization techniques
- Use of unstructured meshes
- Fictitious Boundary (FBM) methods
- Newton-Multigrid solvers
- Parallel (domain decomposition)

**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 (Level Set)
- \(s/l\) interface capturing method (FBM)
- \((s,l)/l/g\) composite jets of \(l/l\) and/or \(s/l\)

**Engineering aspects:**
- Geometrical design
- Modulation strategy
- Optimization

**ALE based mesh deformation:**
- Fast, due to PDE free implementation
- Use of monitor function (distance, gradients, triangulation)
- Dynamic performance for transient problems
- Artificial solver acceleration due to the reduced computational cost w.r.t. the given interface resolution

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

High order Q2 discretization of the Level Set equation

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

Stability requirement: \( \phi \) should be smooth!

Reinitialization / Accurate distance computation / Interface reconstruction

The key is to fully exploit the high order resolution of the interface

- Triangulation of the arising surface
- Recursive subdivision of interface intersected elements (downward direction)
- Hierarchical storage of triangulated subsets (upward direction)

Reduction to mass of points weighted with their integral area
Practical realization – interface reconstruction

High order Q2 discretization of the Level Set equation
\[ \frac{\partial \phi}{\partial t} + v \cdot \nabla \phi = 0 \]

Stability requirement: \( \phi \) should be smooth!

Reinitialization / Accurate distance computation / Interface reconstruction

The key is to fully exploit the high order resolution of the interface
Validation and convergence of the flow solver

3D Rising Bubble benchmark initiative:

http://wissrech.ins.uni-bonn.de/research/projects/risingbubblebenchmark/

Spatial convergence: FEATFLOW vs Ref

Temporal convergence: FEATFLOW vs Ref  FEATFLOW vs other discret. techniques
Validation of droplet generation w.r.t. experiments

Cooperation with the group of Prof. Walzel / TU Dortmund

\[ \sigma_{CD} = 0.025 \text{ N/m} \ (\pm 0.001 \text{ N/m}) \]

\[ \mu_1 : \mu_2 \approx 1.0 \]

\[ \rho_1 : \rho_2 \approx 1.0 \]

• Dripping shows an excellent agreement with experiments
• Increasing sensitivity of the process for higher flowrates leading to jetting!
• Introduction of controlled source of disturbances in terms of modulation

\[ \frac{V_D}{V_C} = 2.5:123.1 \]

\[ \frac{V_D}{V_C} = 3.0:148.7 \]

\[ \frac{V_D}{V_C} = 4.0:197.0 \]
Recent development: Grid deformation and ALE

Advantages:

- Constant mesh/data structure
- Increased resolution in regions of interest
- Nonlinear PDE approach is **not** necessary → anisotropic Laplace smoother
- Straightforward usage for 3D unstructured meshes

Intelligence of the method depends on the construction of the monitor function

- Geometrical description (solid body, interface triangulation)
- Field oriented description (steep gradients, fronts) → numerical stabilization

Microfish dynamics
Cooperation with:
Prof. Fischer @ MPI IS Stuttgart
Work published in:
Nature Communications, 2014

Twinscrew extruders
Cooperation with:
Prof. Schöppner @ KTP Paderborn
Work submitted to:

Microreactors
Cooperation with:
Prof. Schlüter @ TUHH Hamburg

Computational mesh after deformation
Simulation of viscous liquid jets

J. M. Nóbrega et al.: The phenomenon of jet buckling: Experimental and numerical predictions

Corn syrup - air system

24x24x48 mesh

Interface triangulation:
T₀: ~100,000 triangles
Tₙ: ~300,000 triangles

Rendering: Raphael Münster / Blender
Encapsulation via modulation

Reference case:
Newtonian inner/outer liquid

Physical parameters for the simulation set-up:
\[ \mu_1 : \mu_2 : \mu_3 = 1 : 100 : 100 \]
\[ \rho_1 : \rho_2 : \rho_3 = 1 : 1000 : 1000 \]
\[ \sigma_{12} : \sigma_{23} = 1 : 1 \]
\[ \dot{V}_2 : \dot{V}_3 = 1 : 3.5 \]
Encapsulation via modulation
Reference case Newtonian inner/outer liquid

Triangulation oriented mesh deformation
Encapsulation via modulation

Influence of the mesh resolution → mesh convergence

~30% less surface resolution in a $1.5^3$ larger domain
Encapsulation via modulation
Non-Newtonian shell / Newtonian core material

Viscosity model:
Shear thinning power law:
\[ \mu = \mu_0 (\varepsilon + \dot{\gamma})^{n-1} \]
where
\[ \dot{\gamma} = \| D(u) \| = \left\| \frac{1}{2} [\nabla u + (\nabla u)^T] \right\| \]
\[ \varepsilon = 10^{-4} \]

Increasing shear thinning effects leading to suppressed satellite droplet formation

Solver adjustments
- Fixed point iteration for the nonlinearity
- Defect evaluation with the deformation tensor
- Preconditioned with shear dependent diff. operator

Viscosity distribution in the laminar jet (n=0.8)
Conclusions

- ALE based grid deformation guarantees a **speedup** equivalent to one resolution level (that corresponds to 8 times better performance compared to a static mesh simulation with a comparable resolution)
- High order discretization together with the developed reinitialization procedure guarantees excellent mass conservation and convergence properties
- The simulation tool has been validated in a sequence of stages of development
- The developed production code is configured for realistic encapsulation processes

Outlook

Encapsulation in the framework of fluids obeying more specific rheological models:
- Viscoelastic fluids (single phase with LCR is already implemented)
- Viscoelastic fluids (cooperation with Prof. Frigaard @ Vancouver)
Thank You for Your attention