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Validierung einer Phasenfeldmethode für die Zerteilung einer aufsteigenden Blase durch einen horizontalen Zylinder

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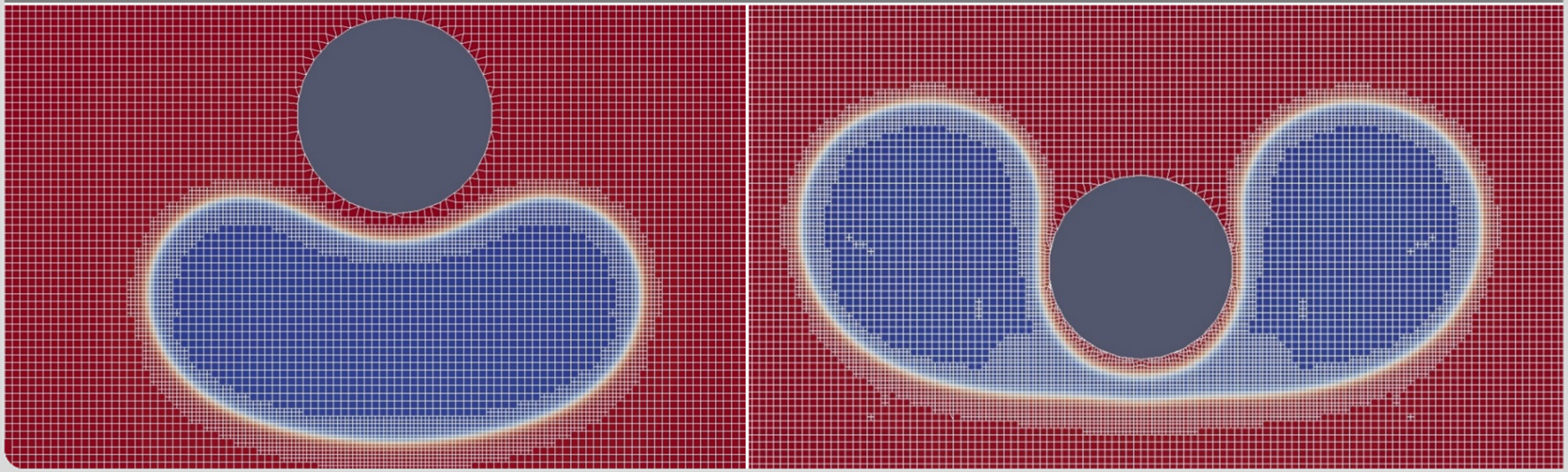
[4] Karlsruher Institut für Technologie (KIT), Institut für Katalyseforschung und –technologie (IKFT), Karlsruhe, Deutschland

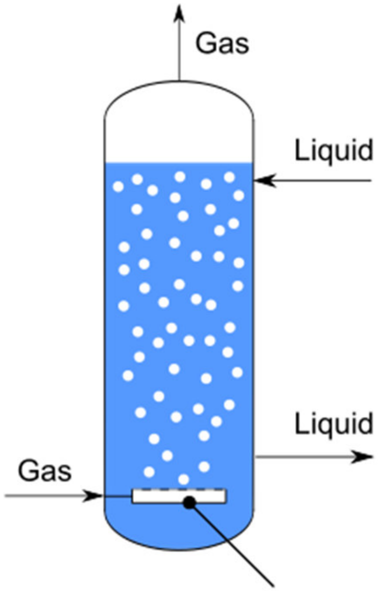
Jahrestreffen der ProcessNet-Fachgruppe CFD, Frankfurt am Main, 19.-20. März 2019



Outline

- Introduction
  - Background
  - Motivation and goal
- Numerical method
  - Phase-field method in OpenFOAM-extend
  - Validation by bubble rise benchmark from literature
- Interaction between rising bubble and horizontal cylinder
  - Experiment for validation
  - Simulation results
- Conclusions

Bubble column reactors



wikipedia.org

Production of 600,000 t/a phenol in 15 bubble columns by INEOS Phenol, Gladbeck, Germany

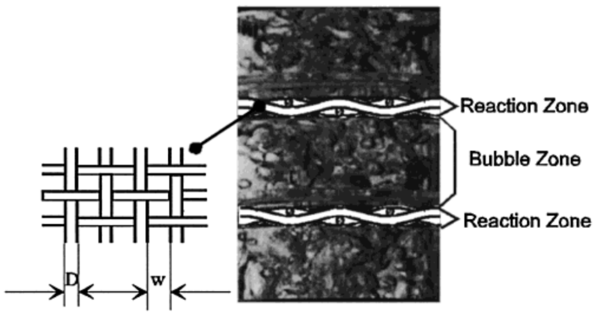


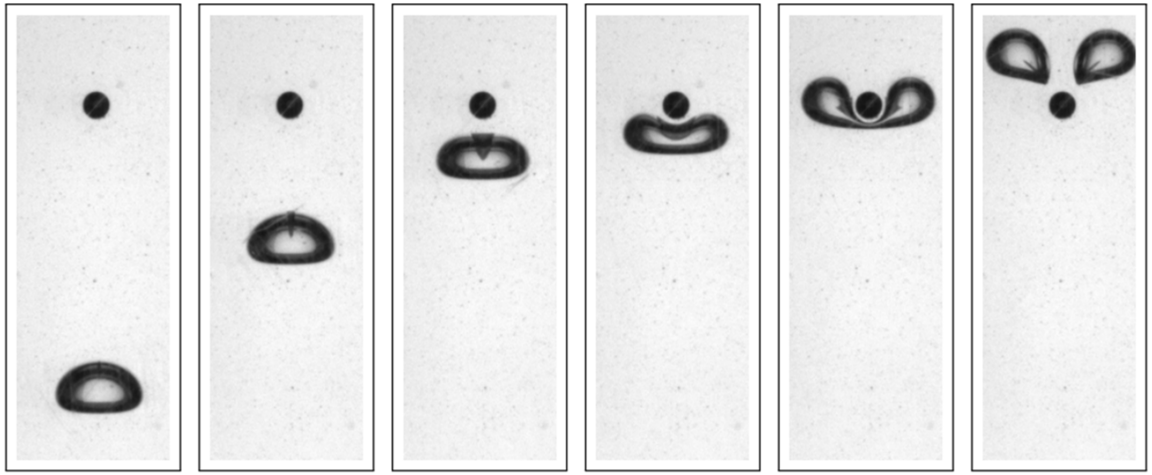
Figure 1. Bubble column staged with structured fibrous catalysts.

- Reactor internals serve to fragment bubbles and increase interfacial area
- Wire meshes serve as catalyst support
- **Does the interaction between bubbles and mesh depend on wire wettability?**

V. Höller, K. Radevik, L. Kiwi-Minsker, A. Renken, *Ind. Eng. Chem. Res.* **40** (2001) 1575–1579

EU project “Cutting Bubbles”

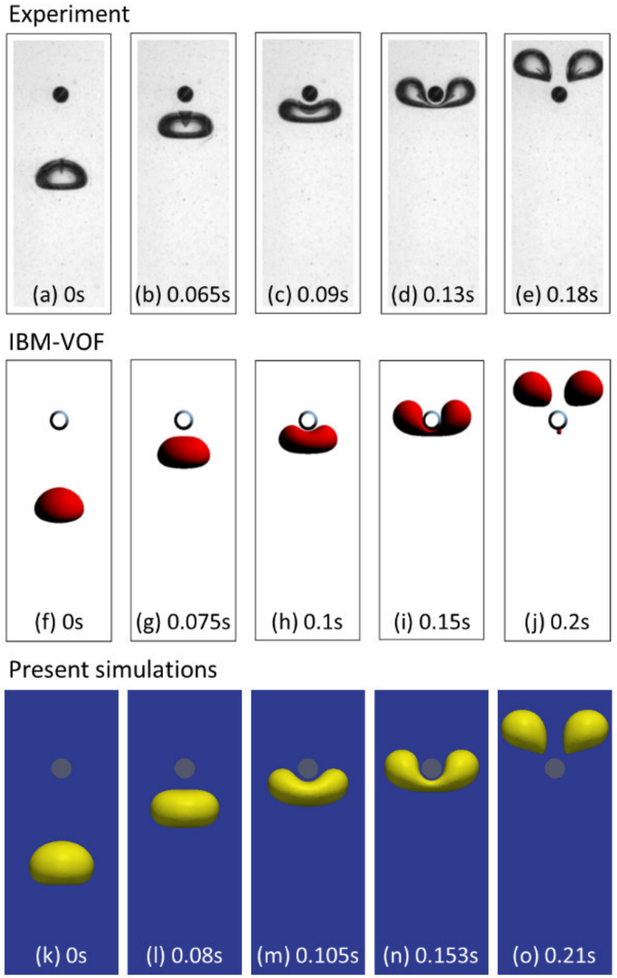
- ERC starting grant Niels Deen TU Eindhoven (2010-2015)
  - Experiments and simulations for various scales and flow conditions
  - Sulzer packing – wire meshes – **single wire/cylinder**
  - Influence of structure/wire wettability was not addressed
- Experiments by Q. Segers (2015)
  - Cutting of a rising bubble by a horizontal cylinder



Stainless steel cylinder 3 mm in diameter

📖 Q. Segers, Cutting Bubbles using Wire-Mesh Structures - Direct Numerical Simulations, PhD thesis, TU Eindhoven 2015

Interface-resolving simulations



Experiment Segers (2015)

VOF simulations (Baltussen et al. 2017)

No specific conditions for contact angle

Phase field simulations (Cai et al. 2016)

Static contact angle $\theta_s = 60°$

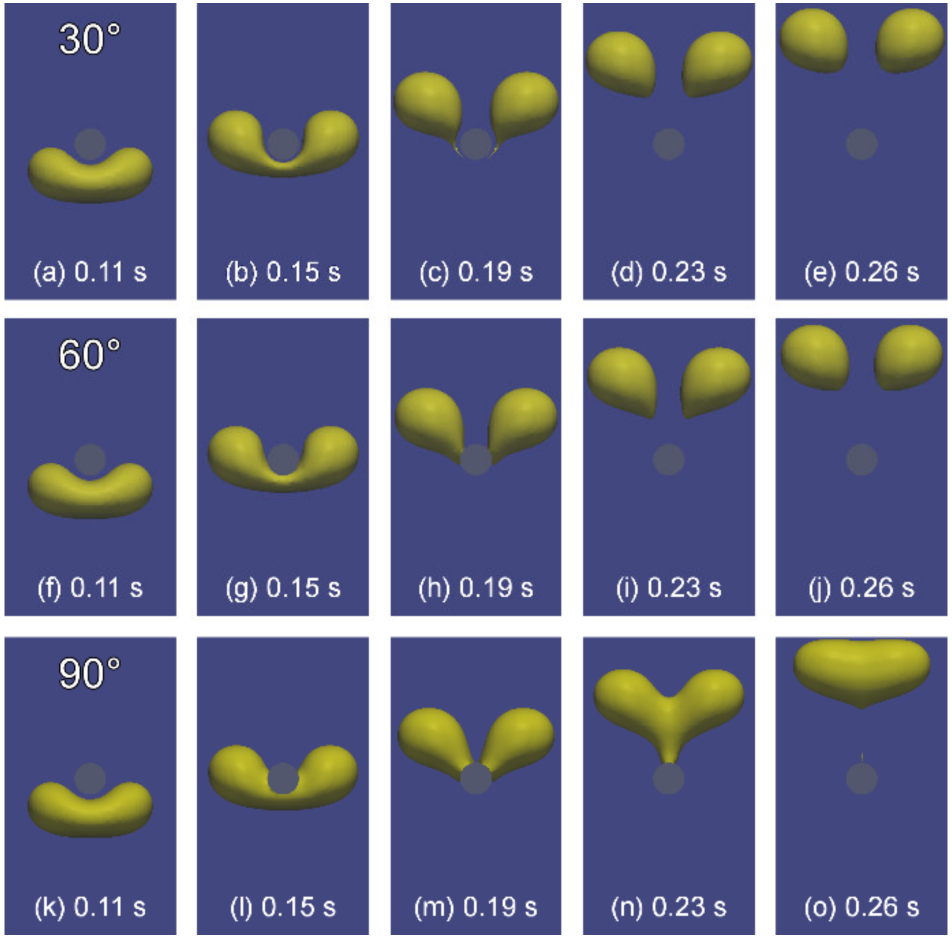
← *Time in figures is slightly different*

📖 Q. Segers, Cutting Bubbles using Wire-Mesh Structures - Direct Numerical Simulations, PhD thesis, TU Eindhoven 2015

📖 M. Baltussen, Q. Segers, J. Kuipers, N. Deen, *Chem. Eng. Sci.*, **157** (2017) 138–146

📖 X. Cai, M. Wörner, H. Marshall, O. Deutschmann, *Catalysis Today* **273** (2016) 151–160

Influence of cylinder wettability



- Simulation results for θ_s = 90° are predictions
  - Lack of experiments for cylinders with different wettability
- <u>Goal</u>
  - Perform experiments
  - Validate computer code *PhaseFieldFoam*

📖 X. Cai, M. Wörner, H. Marshall, O. Deutschmann, *Catalysis Today* **273** (2016) 151–160

Outline

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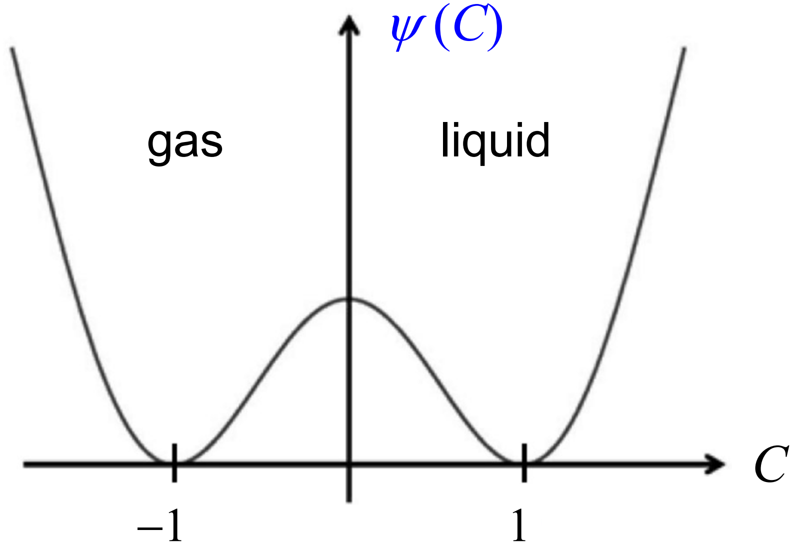
Phase-field method

- Free energy of two-phase mixture (m = mixture) [J]

$$\mathcal{F}_{\mathrm{m}} = \int_{\Omega} f_{\mathrm{m}}(C, \nabla C)\,\mathrm{d}\Omega$$

$$f_{\mathrm{m}}(C, \nabla C) = \underbrace{\frac{\lambda}{\varepsilon^2}\psi(C)}_{\text{bulk energy}} + \underbrace{\frac{\lambda}{2}|\nabla C|^2}_{\text{gradient energy}}$$

$$\underbrace{\psi(C) = \frac{1}{4}(1 - C^2)^2}_{\text{Ginzburg-Landau double-well potential}}$$



  - C = order parameter [-]
  - ε = capillary width [m]
  - λ = mixing energy density [J/m]
  - f_{m} = free energy density [J/m^3]

Equilibrium profile

- Bulk chemical potential [J/m³]

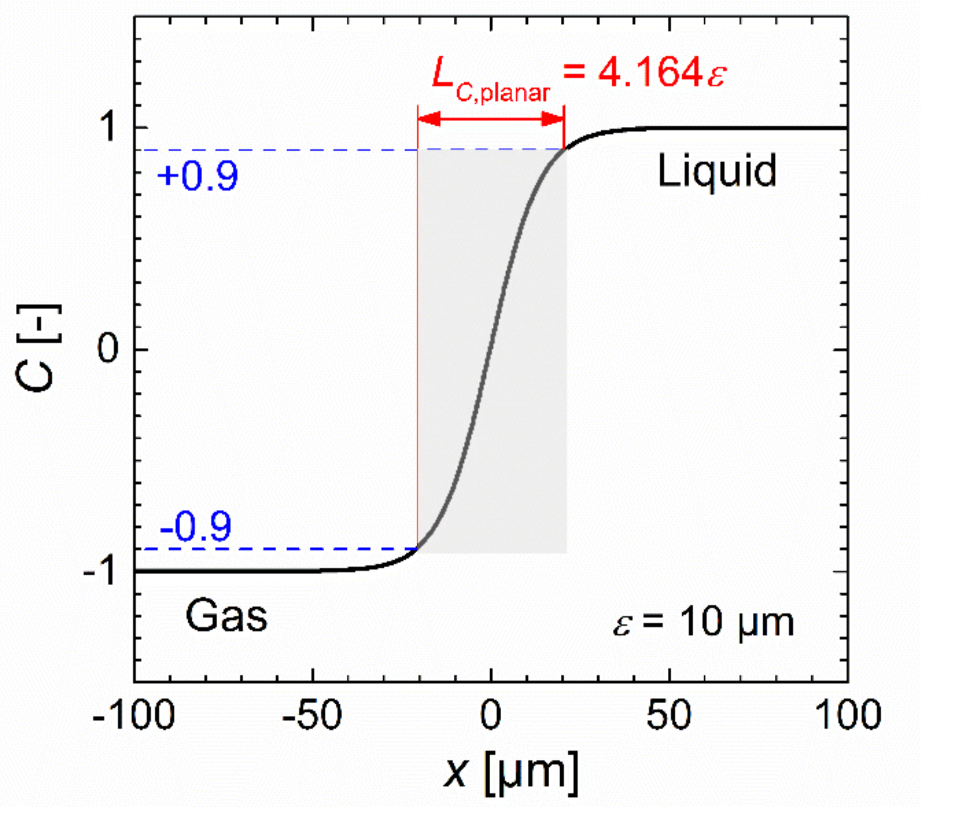
$$\phi_{\mathrm{m}} = \frac{\delta \mathcal{F}}{\delta C} = \lambda \varepsilon^{-2} \underbrace{(C^3 - C)}_{=\psi'} - \lambda \nabla^2 C$$

- 1D equilibrium profile

$$C(x) = \tanh\left(\frac{x}{\sqrt{2}\varepsilon}\right)$$

- Interfacial tension

$$\sigma = \int_{-\infty}^{\infty} \lambda \left(\frac{\mathrm{d}C}{\mathrm{d}x}\right)^2 \mathrm{d}x = \frac{\sqrt{8}}{3}\frac{\lambda}{\varepsilon}$$



Wetting boundary condition

- Free energy at solid wall [J]

$$\mathcal{F}_{\mathrm{w}} = \int_{\partial\Omega_{\mathrm{w}}} f_{\mathrm{w}}(C)\mathrm{d}A$$

- Free energy density of wall (static contact angle θ_{s})

$$f_{\mathrm{w}}(C) = -\frac{\sigma}{4}(3C - C^3)\cos\theta_s + \frac{\sigma_{\mathrm{w1}} + \sigma_{\mathrm{w2}}}{2}$$

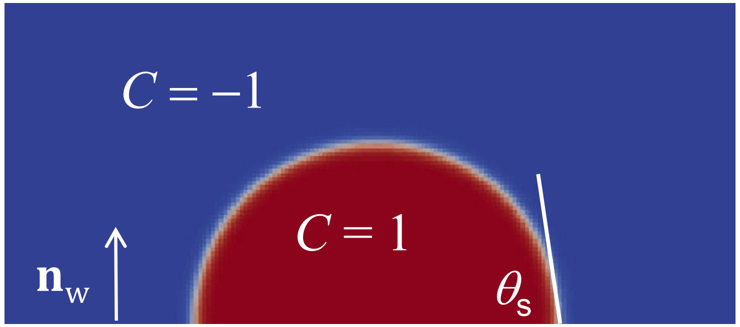
$$\underbrace{\sigma_{\mathrm{w2}} - \sigma_{\mathrm{w1}} = \sigma\cos\theta_{\mathrm{s}}}_{\text{Youngs equation}}$$

- Wall chemical potential [J/m²]

$$\phi_{\mathrm{w}} = \frac{\delta\mathcal{F}_{\mathrm{w}}}{\delta C} = \lambda\mathbf{n}_{\mathrm{w}}\cdot\nabla C - \frac{3}{4}\sigma(1 - C^2)\cos\theta_{\mathrm{s}}$$

- Equilibrium condition

$$\mathbf{n}_{\mathrm{w}}\cdot\nabla C = \partial_{n,\mathrm{w}}C = \frac{1 - C^2}{\sqrt{2}\varepsilon}\cos\theta_{\mathrm{s}}$$



Cahn-Hilliard equation

- Convective Cahn-Hilliard equation

$$\partial_t C + \nabla\cdot(C\,\mathbf{u}) = M\nabla^2\phi_\mathrm{m} \qquad \phi_\mathrm{m} = \lambda\varepsilon^{-2}(C^3 - C) - \lambda\nabla^2 C$$

  - $\mathbf{u}$ = velocity field [m/s]
  - M = constant mobility parameter [m^{3}s/kg]
- Boundary conditions
  - Zero gradient of chemical potential $\partial_n\phi_\mathrm{m} = 0$
  - Wettability condition at wall $\partial_{n,\mathrm{w}} C = 2^{-1/2}(1 - C^2)\varepsilon^{-1}\cos\theta_\mathrm{s}$
- No-slip condition for velocity field
  - Diffusive mechanism for motion of the contact line

$$\mathbf{u}_\mathrm{w} = \mathbf{0} \quad\rightarrow\quad \partial_t C = M\nabla^2\phi_\mathrm{m}$$

📖 J.W. Cahn, J.E. Hilliard, *J. Chem. Phys.* **28** (1957) 258–267

Single field Navier-Stokes equations

- Two incompressible Newtonian fluids

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

$$\partial_t(\rho_C\mathbf{u})+\nabla\cdot(\rho_C\mathbf{u}\otimes\mathbf{u})=-\nabla p+\nabla\cdot\left[\mu_C\left(\nabla\mathbf{u}+(\nabla\mathbf{u})^{\mathrm{T}}\right)\right]+\rho_C\mathbf{g}+\mathbf{f}_\sigma$$

$$\rho_C=\frac{1+C}{2}\rho_{\mathrm{L}}+\frac{1-C}{2}\rho_{\mathrm{G}},\quad \mu_C=\frac{1+C}{2}\mu_{\mathrm{L}}+\frac{1-C}{2}\mu_{\mathrm{G}},\quad \mathbf{f}_\sigma=-C\nabla\phi_{\mathrm{m}}$$

- Determining the phase field parameters ε, λ, M
  - Cahn number $Cn=\varepsilon/L=\mathcal{O}(10^{-2})$
    - L = characteristic macroscopic length scale (here bubble diameter)
  - Mixing energy parameter $\lambda=3\varepsilon\sigma/\sqrt{8}$
  - Mobility parameter $M=\chi\varepsilon^2$
    - Proportionality factor χ [m·s/kg] $\chi=\mathcal{O}(10^{-1}-10^{1})$

D. Jacqmin, *J. Comput. Phys.* **155** (1999) 96–127

J. Kim, *Commun. Comput. Phys.* **12** (2012) 613–661

Computer code *phaseFieldFoam*

- Code development
  - H. Marschall (TU Darmstadt), X. Cai (KIT, now Bosch), …
- Implementation in OpenFOAM-extend
  - foam-extend-1.6, foam-extend-3.2, foam-extend-4.0
  - Finite volume method on general grids
  - Cahn-Hilliard or Allen-Cahn approach
  - Segregated or coupled solution of CH-NS equations
  - PISO/PIMPLE algorithm for pressure-velocity coupling
  - 2nd order schemes in space and time
- Validation and application for various test cases
  - Low spurious currents which converge under mesh refinement

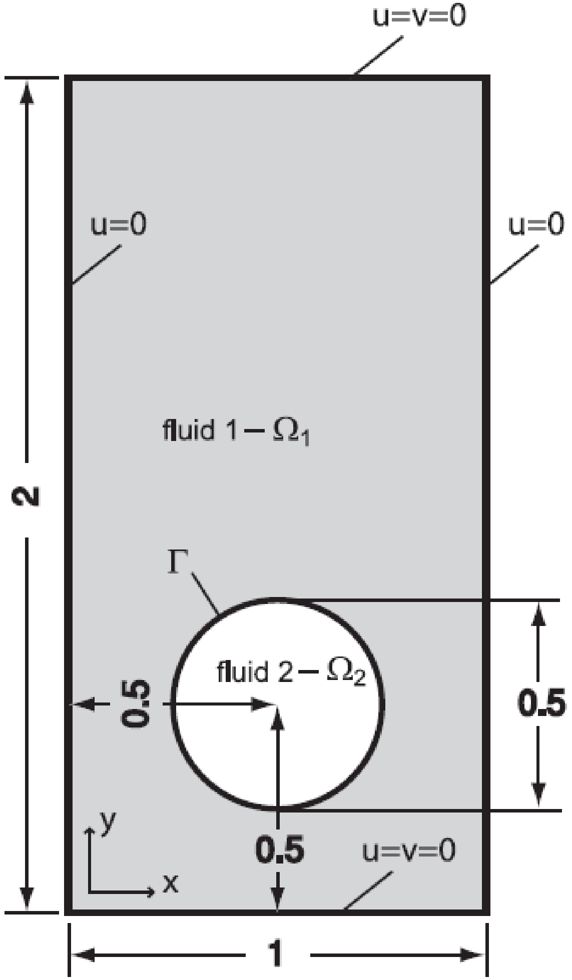
📖 X. Cai, H. Marschall, M. Wörner, O. Deutschmann, *Chem. Eng. Technol.* **38** (2015) 1985–1992

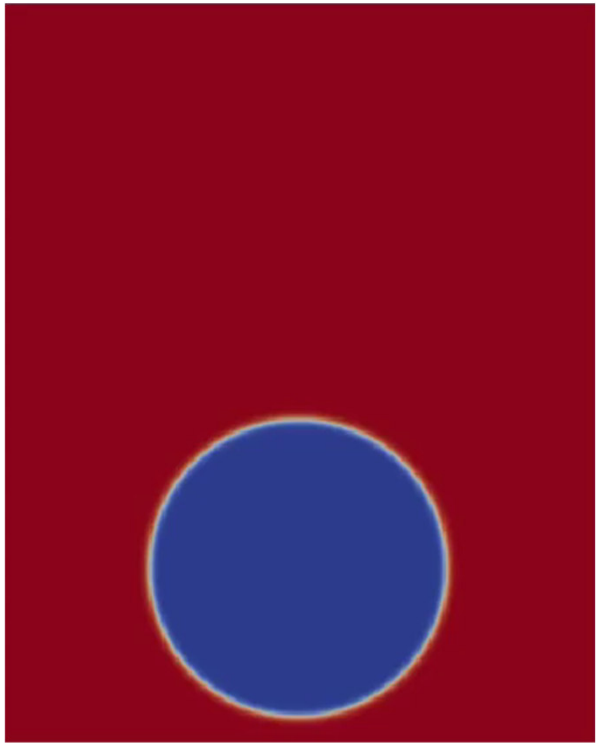
📖 X. Cai, M. Wörner, H. Marschall, O. Deutschmann, *Catalysis Today* **273** (2016) 151–160

📖 X. Cai, M. Wörner, H. Marschall, O. Deutschmann, *Emission Control Science and Technology* **3** (2017) 289–301

📖 F. Jamshidi, H. Heimel, M. Hasert, X. Cai, O. Deutschmann, H. Marschall, M. Wörner, *Comp. Phys. Commun.* **236** (2019) 72–85

Planar bubble rise benchmark



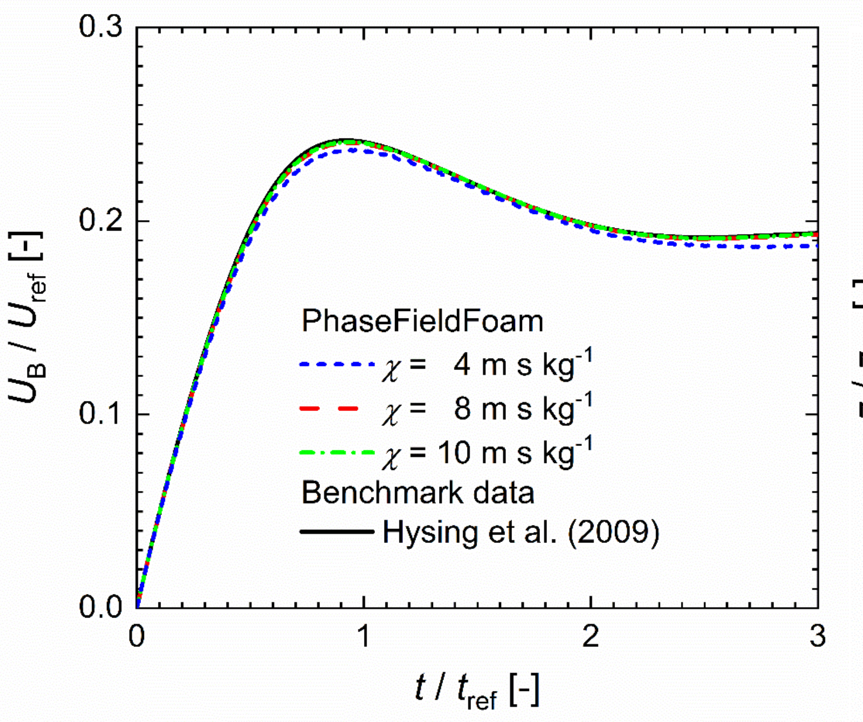


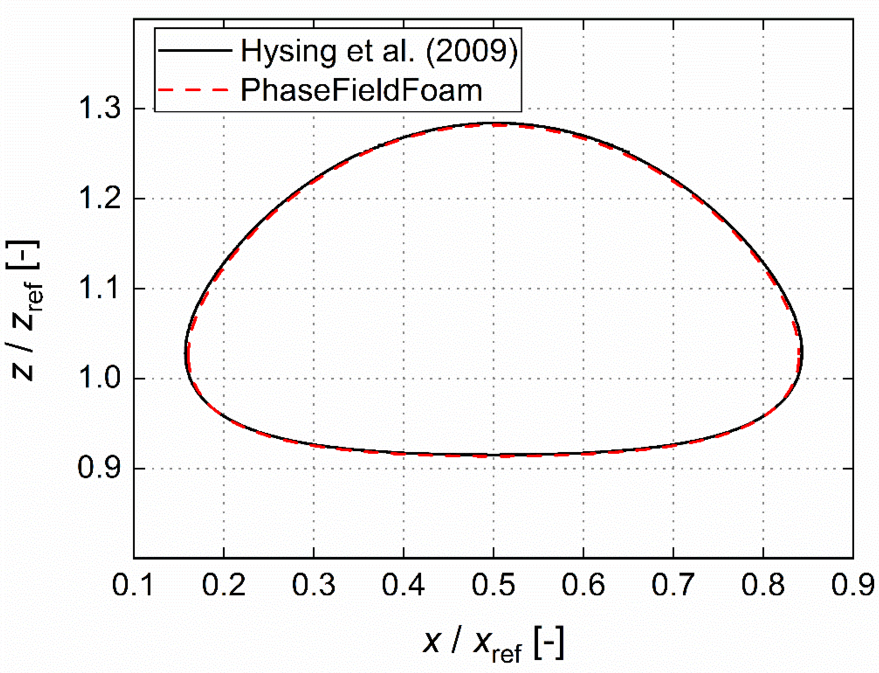
(detail)

S. Hysing, S. Turek, D. Kuzmin, N. Parolini, E. Burman, S. Ganesan, L. Tobiska, *Int. J. Num. Meth. Fluids* **60** (2009) 1259–1288

Planar bubble rise benchmark

- Cn = 0.01, $h = \varepsilon / 2 \rightarrow N_{di}$ = 8 cells in diffuse interface, grid 400×800
- Slight influence of mobility on bubble rise velocity
- Good agreement of bubble shape for $t / t_{ref} = 3$





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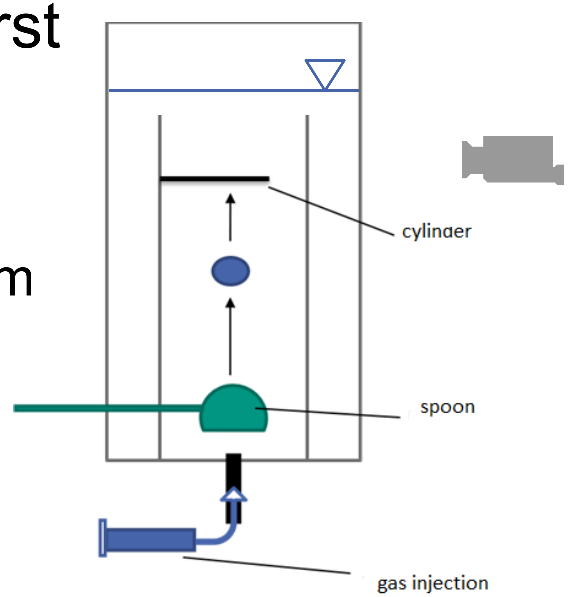
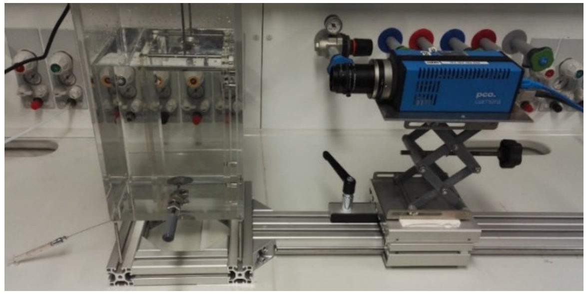
Bubble cutting experiments

- Experiments by P. Rohlfs and M. Börnhorst
  - Set-up similar to Segers (2015)
- Viscous glycerol-water solution (90 w%)
  - ρ_L = 1233 kg/m^3, μ_L = 0.156 Pa s, σ = 66 mN/m
  - Morton number 0.0164
- Cylinders of different material and size
  - Glass, stainless steel, Teflon (θ_s = 40 – 150°)
  - Diameter d_{cyl} = 3 – 5 mm
- Bubble volume V_B = 50 – 1000 µL
  - Equivalent diameter d_B = 4.57 – 12.4 mm
  - Eötvös number 3.8 – 27.3
- Recording by high-speed camera





📖 P. Rohlfs, Einfluss des Benetzungsverhaltens auf die Blasenzerteilung an einem Zylinder, Bachelor thesis, KIT 2018
📖 Q. Segers, Cutting Bubbles using Wire-Mesh Structures - Direct Numerical Simulations, PhD thesis, TU Eindhoven 2015

Hollow glass cylinder d_{cyl} = 4 mm, $\theta_s \approx 40°$

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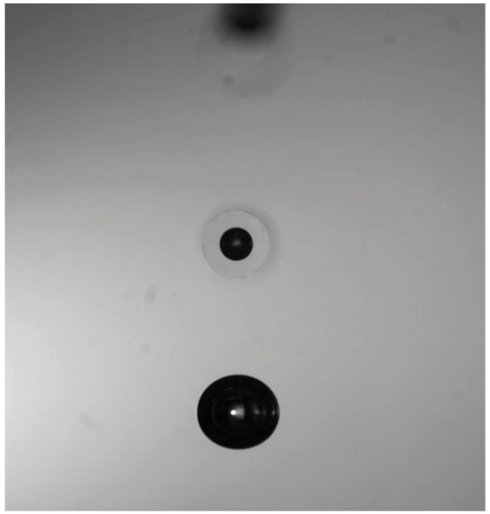
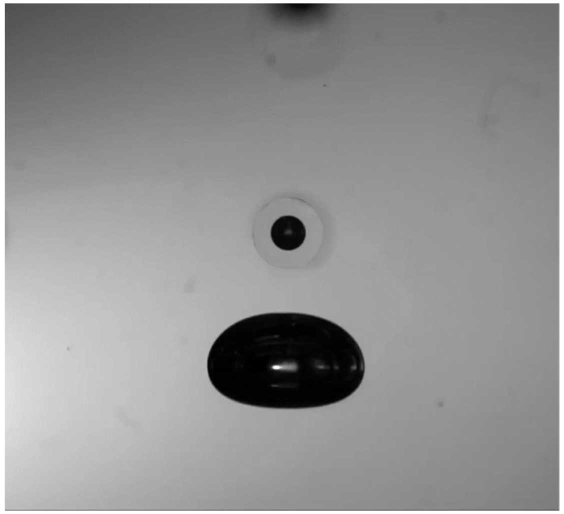
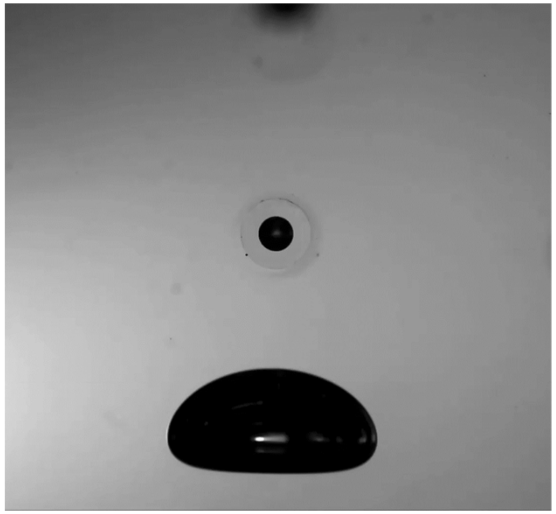
V_B = 50 µL d_B = 4.57 mm	**V_B = 250 µL** d_B = 7.82 mm	**V_B = 500 µL** d_B = 9.85 mm







Bubble slips off	Breakup in two daughter bubbles	Breakup in daughter and satellite bubbles

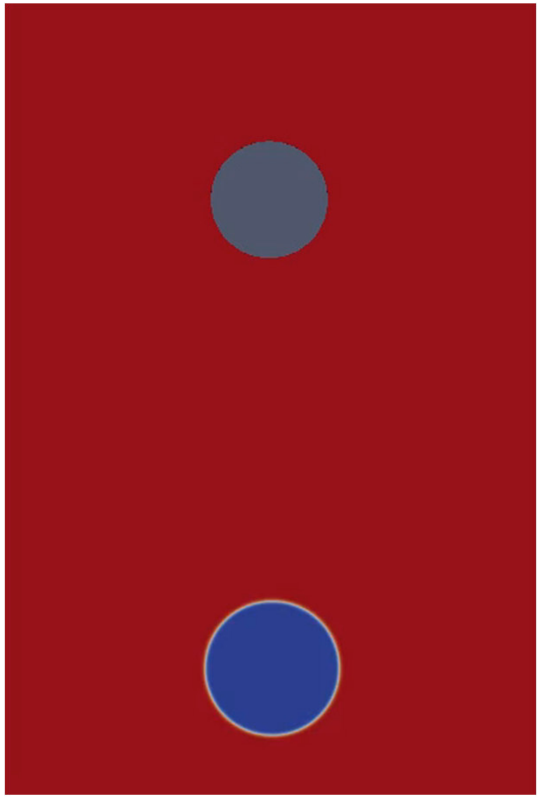
📖 P. Rohlfs, Einfluss des Benetzungsverhaltens auf die Blasenzerteilung an einem Zylinder, Bachelor thesis, KIT 2018

Simulation setup and strategy

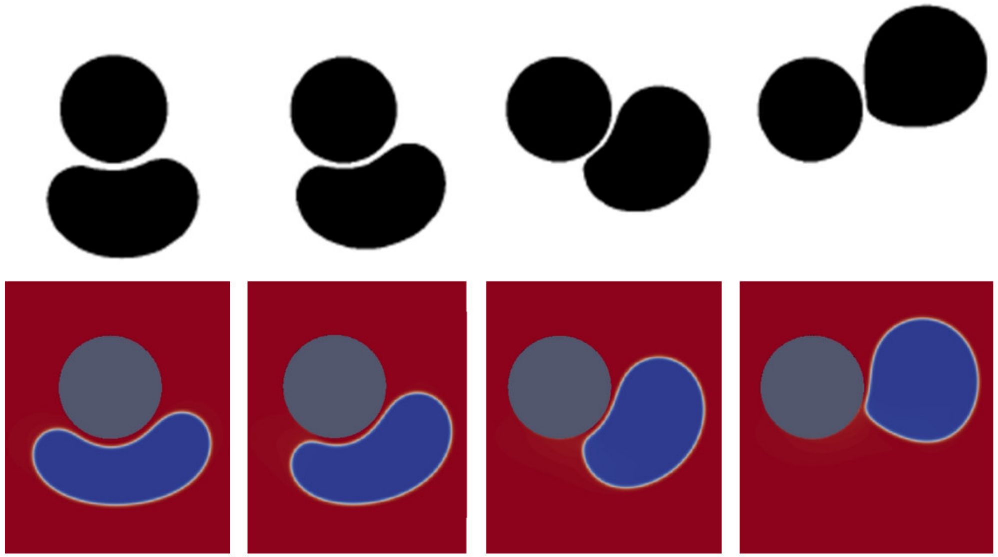
- Parameters taken from experiment
  - Physical properties
  - Cylinder diameter 4 mm
  - Bubble volumes V_B = 50, 250 and 500 µL
- Numerical parameters
  - Fixed Cahn number $Cn = \varepsilon / d_B = 0.01 \rightarrow \varepsilon = 0.01 d_B$
  - Grid resolution $h = \varepsilon / 2 \rightarrow$ 8 cells in diffuse interface
- Axisymmetric simulation of free bubble rise
  - Determine mobility from measured terminal bubble velocity
  - Estimate distance between initial bubble position and cylinder
- Bubble cutting simulations
  - Planar case for qualitative comparison with experiment
  - 3D case with adaptive mesh refinement for quantitative validation

Planar simulation $A_B = A_{B,50\mu L}$ (θ_s = 60°)

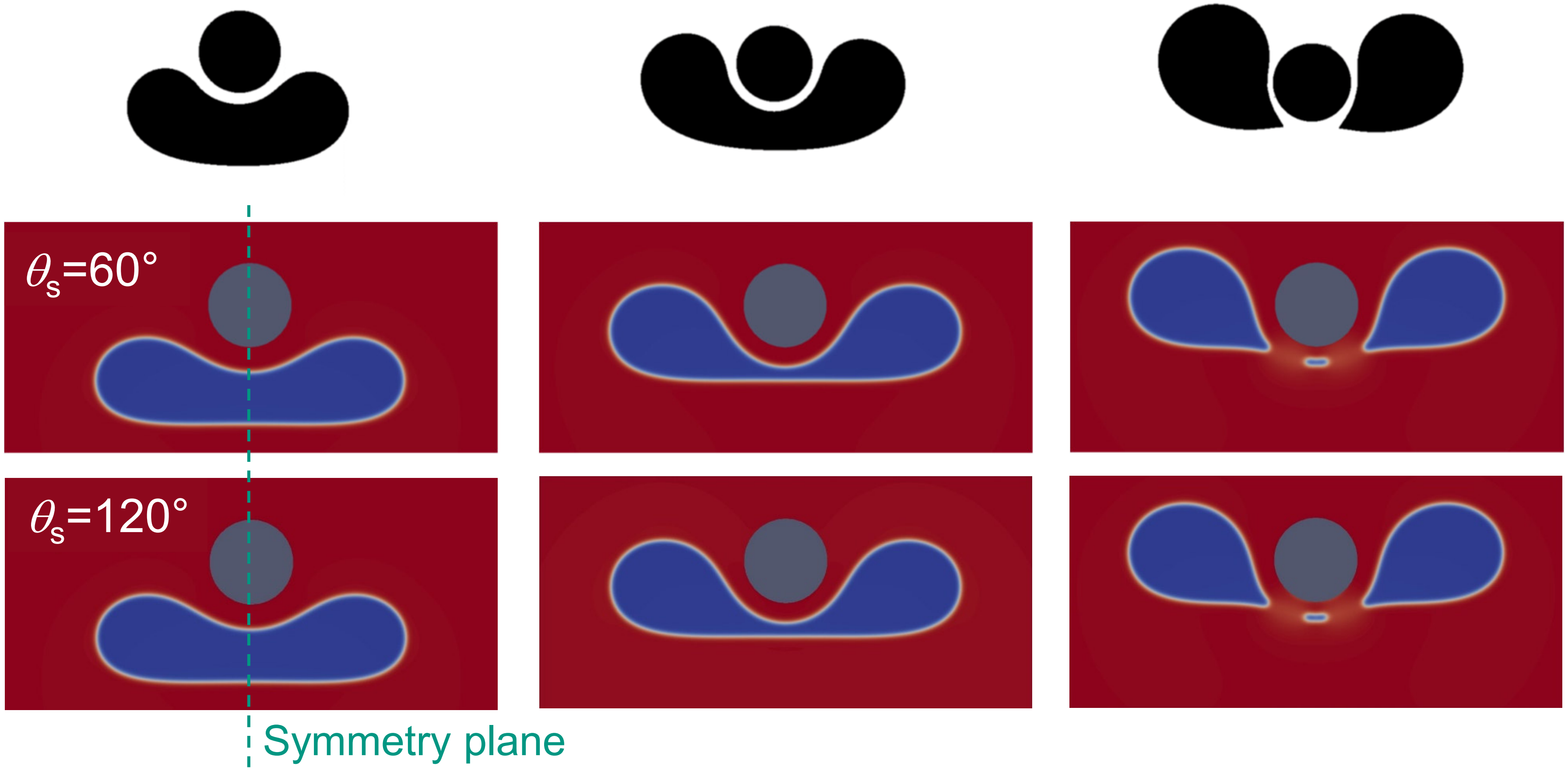
- Slight offset between bubble and cylinder



- Comparison with experiment
  - Qualitative agreement
  - Minimal thickness of liquid film corresponds to about 6ε



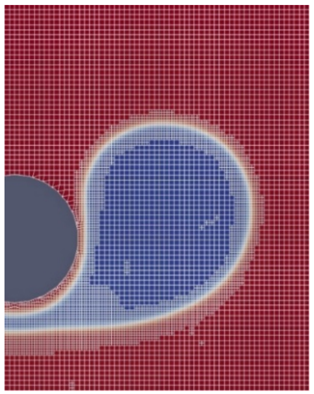
Planar simulation $A_B = A_{B,250\mu L}$

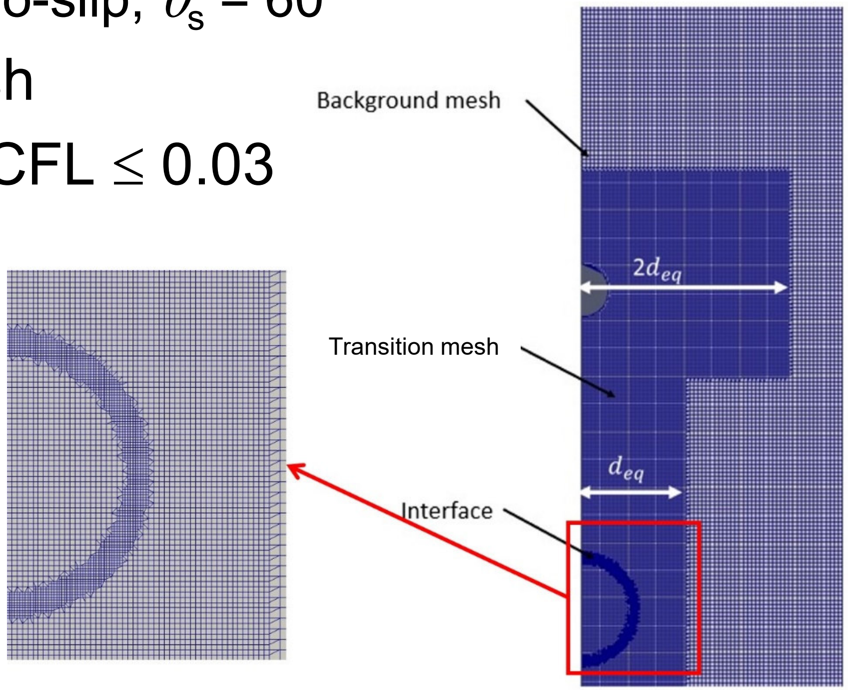


- No contact between gas bubble and cylinder
- Liquid film eliminates influence of cylinder wettability

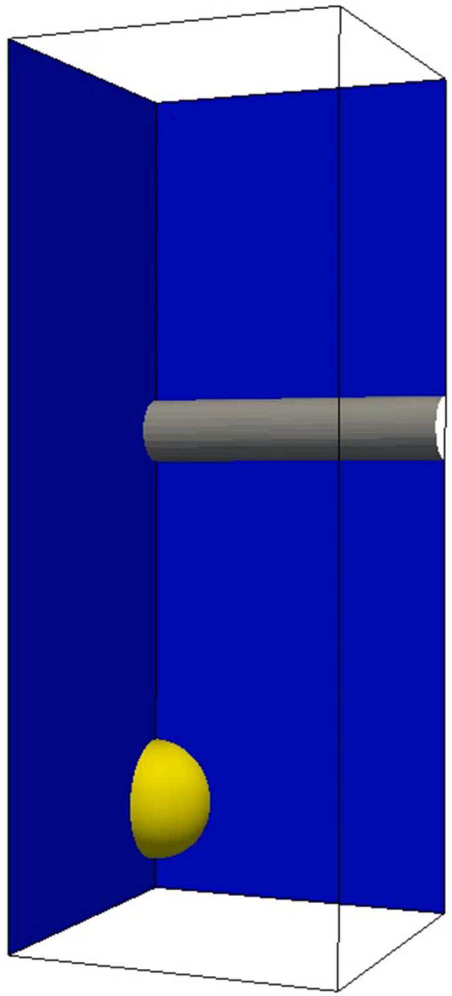
Set-up for 3D simulations

- Boundary conditions
  - Quarter symmetry
  - Free slip at two other lateral boundaries
  - Bottom/top *pressureInletOutletVelocity*
  - Cylinder: no-slip, $\theta_s = 60°$
- Adaptive mesh
- Δt_{max} = 1 µs, CFL $\leq$ 0.03





Initial mesh



V_B = 250 µL (d_B = 7.8 mm)

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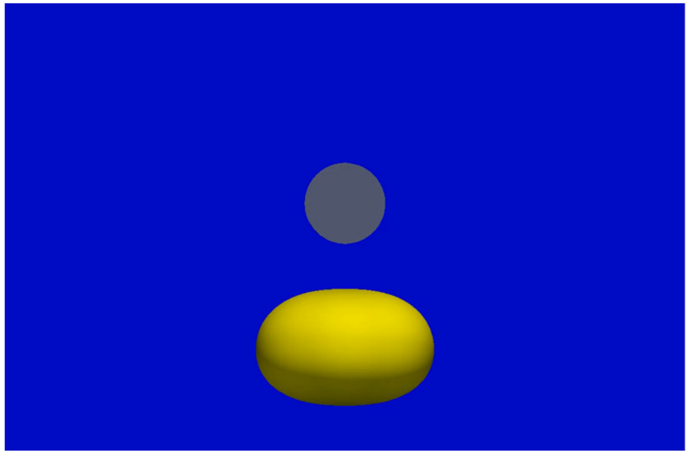
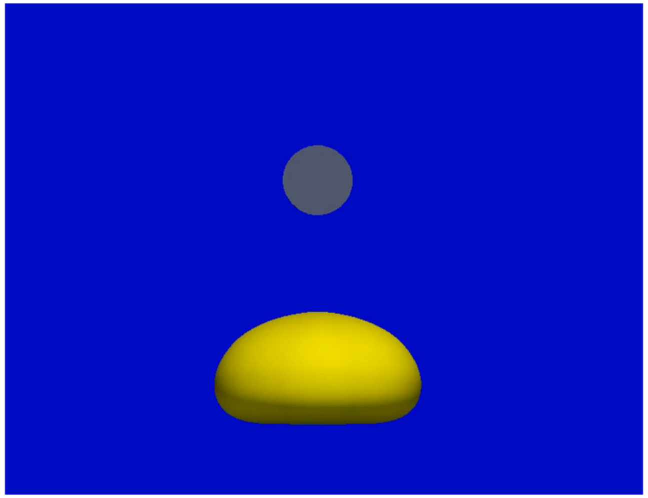
Front view

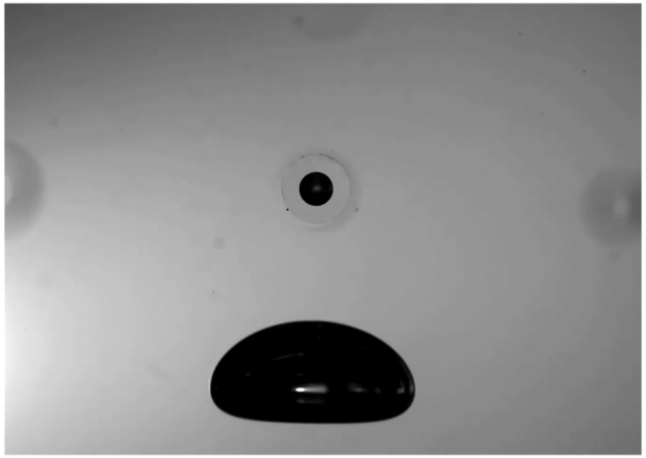


📖 P. Rohlfs, Einfluss des Benetzungsverhaltens auf die Blasenzerteilung an einem Zylinder, Bachelor thesis, KIT 2018
📖 S. Wang, Numerical simulation of the cutting of a rising bubble by a horizontal cylinder, Master thesis, KIT 2019

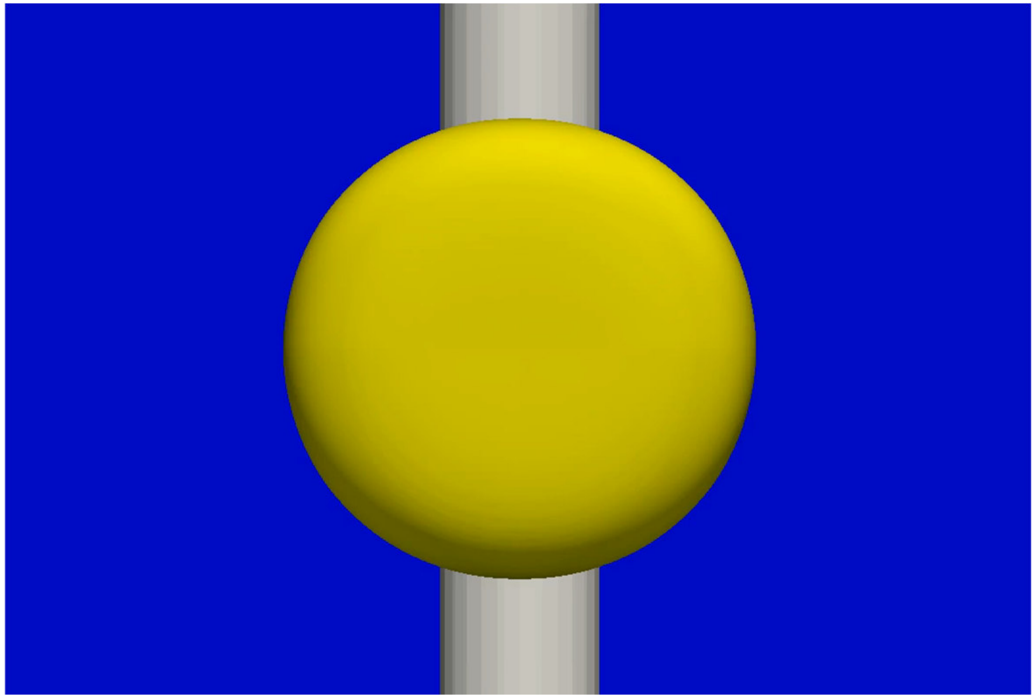
V_B = 500 µL (d_B = 9.8 mm)

Front view





Bottom view



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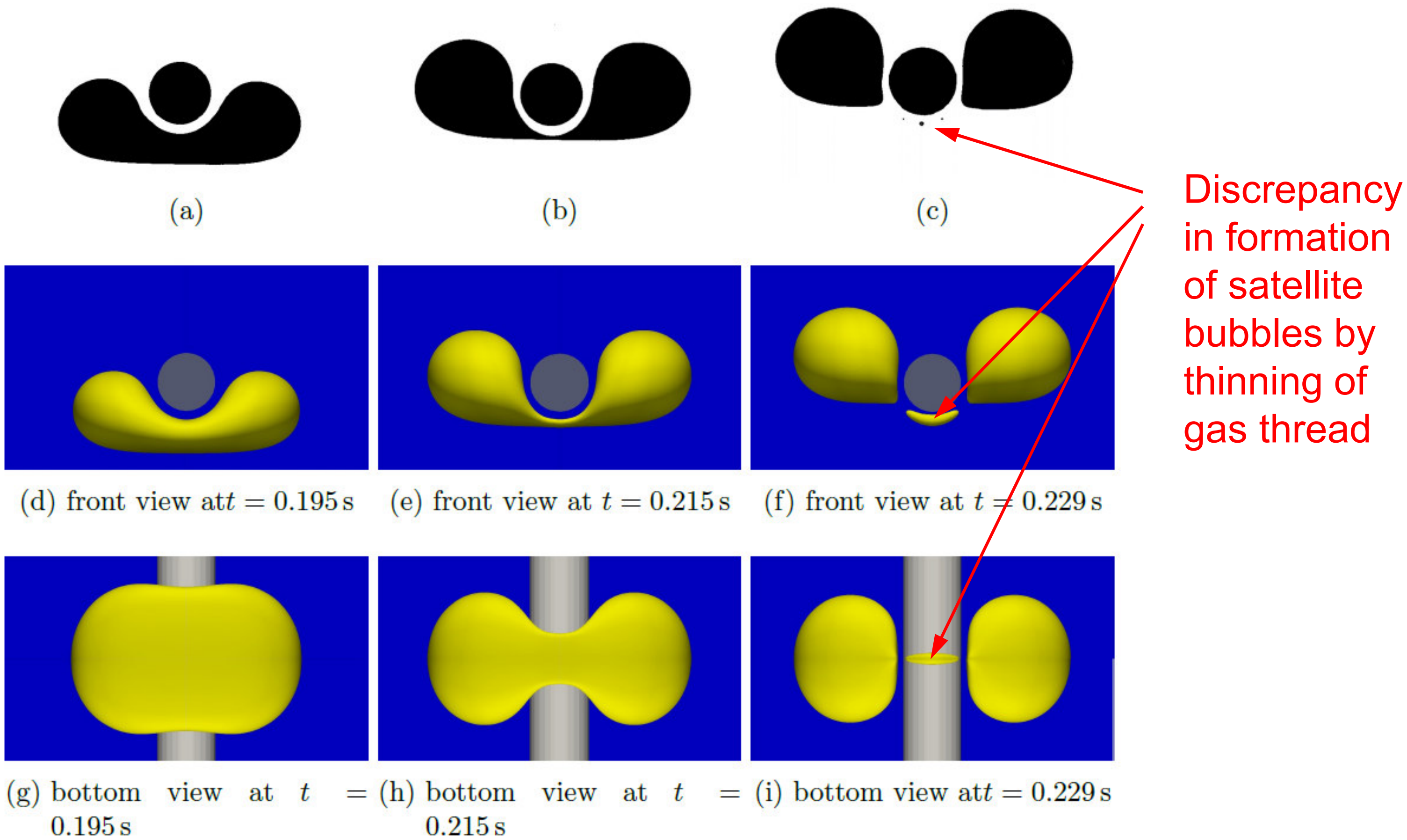
📖 S. Wang, Numerical simulation of the cutting of a rising bubble by a horizontal cylinder, Master thesis, KIT 2019

Exp. ↔ simulation (V_B = 500 µL)

Exp.

Sim.



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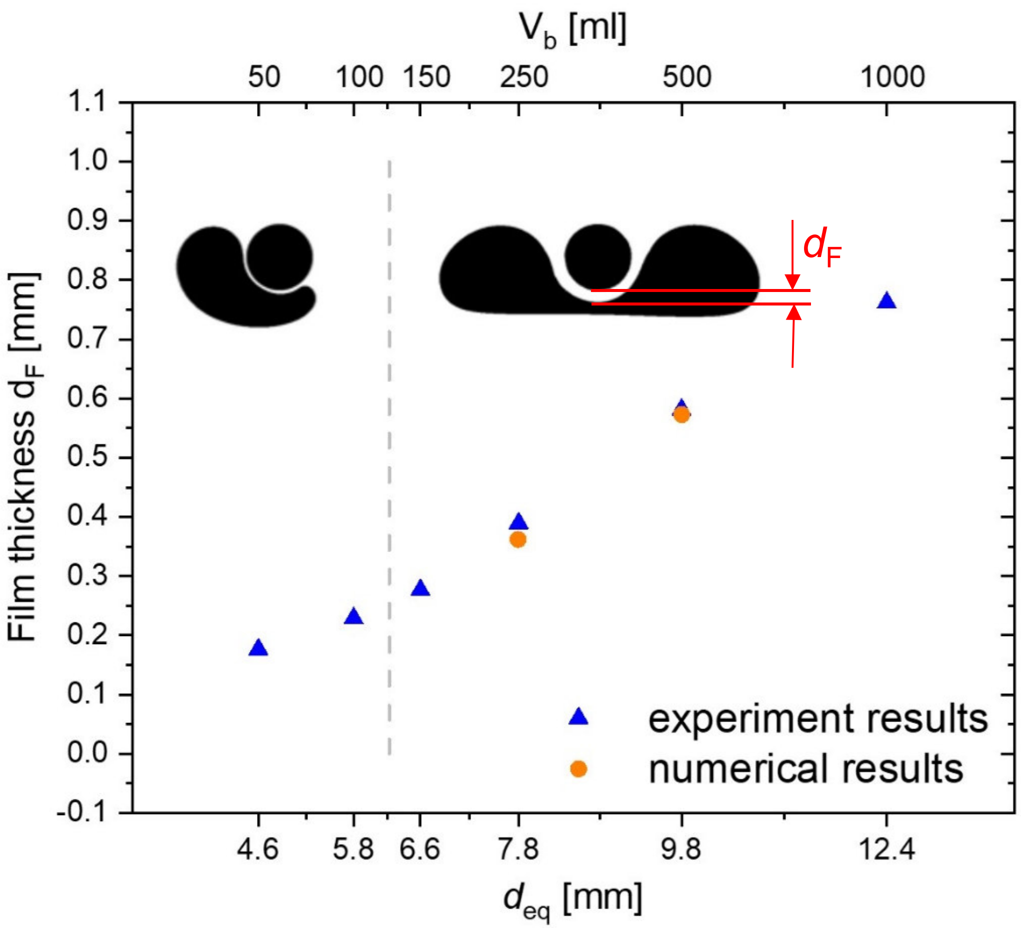
Liquid film thickness d_F vs. V_B



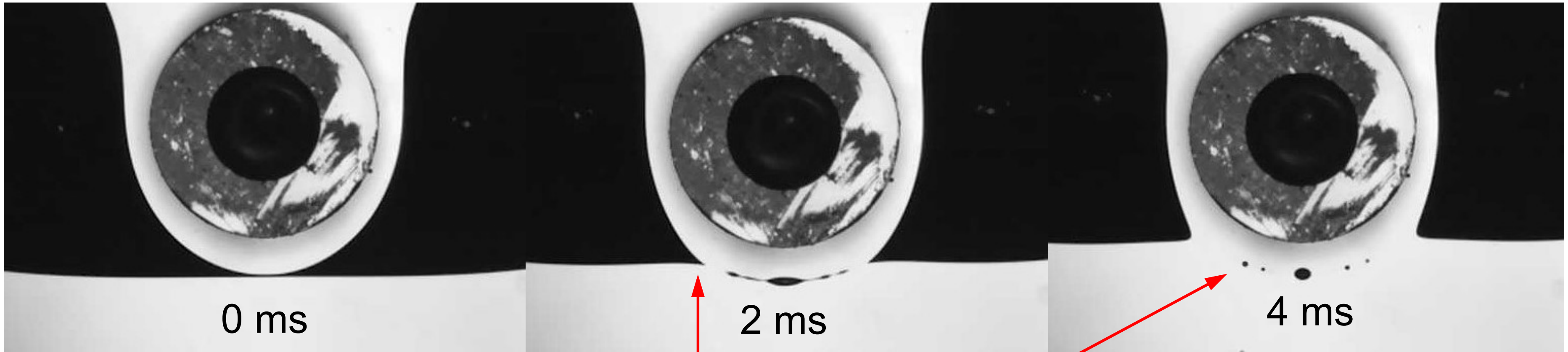
- Bubble and cylinder are always separated by a liquid film
- Thickness d_F of liquid film increases with bubble volume
- Cylinder wettability has no influence on bubble cutting

📖 P. Rohlfs, Einfluss des Benetzungsverhaltens auf die Blasenzerteilung an einem Zylinder, Bachelor thesis, KIT 2018

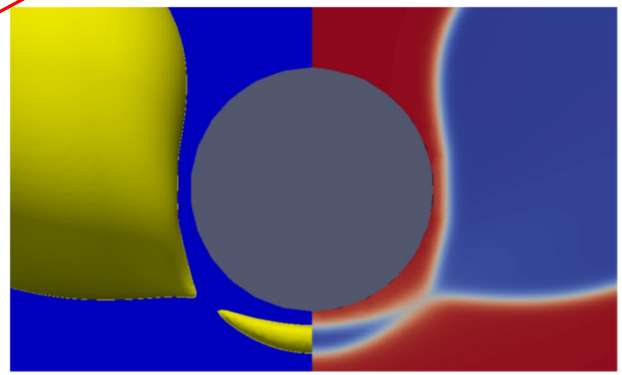
📖 S. Wang, Numerical simulation of the cutting of a rising bubble by a horizontal cylinder, Master thesis, KIT 2019

Formation of satellite bubbles

- Formation of a gas thread between both daughter bubbles
- Thinning and breakup of gas thread (Rayleigh-Plateau inst.)
- Number of SB varies and is not always reproducible



- Numerical challenges
  - Extreme curvature at breakup
  - Tiny satellite bubbles
    $Cn_{SB} = 0.01 \rightarrow \varepsilon = 0.01 d_{SB} \approx 1 \mu m$



Conclusions

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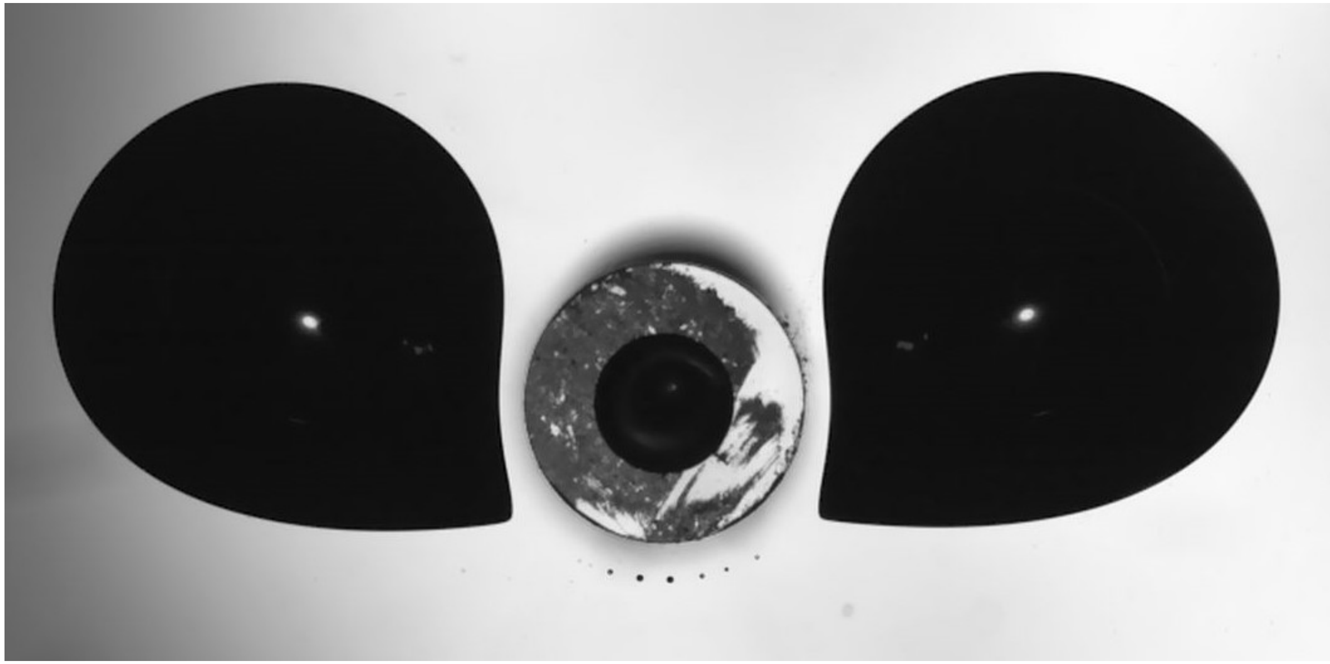
- Phase field method for simulation of gas-liquid flows
  - Coupled Cahn-Hilliard-Navier-Stokes equations
  - Implementation in OpenFOAM-extend (code *phaseFieldFoam*)
  - Mesh independent benchmark results for $Cn \leq 0.01$, $h \leq \varepsilon / 2$
  - Difficulty to choose appropriate value for mobility
- Validation for bubble cutting by horizontal cylinder
  - Bubbles do not come in direct contact with the cylinder
    - Separation by a liquid film (film thickness increases with V_B)
    - Presence of liquid film eliminates effect of cylinder wettability
    - *Observation for present very viscous system, but how in general?*
  - Good agreement for liquid film and daughter bubbles
  - Correct capturing of tiny satellite bubbles forming from thinning gas thread is currently out of reach at least with phase-field method

More about the experiments

M. Börnhorst, T. Homan, P. Rohlfs, N. Deen, O. Deutschmann, M. Wörner
Jahrestreffen Reaktionstechnik 2019 gemeinsam mit der Fachgruppe Mehrphasenströmungen, Würzburg, May 27-29, 2019, Poster

T. Homan, M. Börnhorst, P. Rohlfs, N. Deen, O. Deutschmann, M. Wörner
ICMF, Rio de Janeiro, May 19-24, 2019, Oral presentation



Eight satellite bubbles (V_B=425 µL)

Thank you for your attention

- Acknowledgements

  - B. Frohnapfel & J. Kriegseis from ISTM at KIT (camera for tests)
  - Group of P. Levkin at KIT (hydrophobic coating of glass cylinder)
  - R. Schwarze, J. Klostermann TU Freiberg (Hysing BM with OpenFOAM)
