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ICMF 2016

Numerical study on the wettability dependent interaction of droplets and bubbles with solid structures

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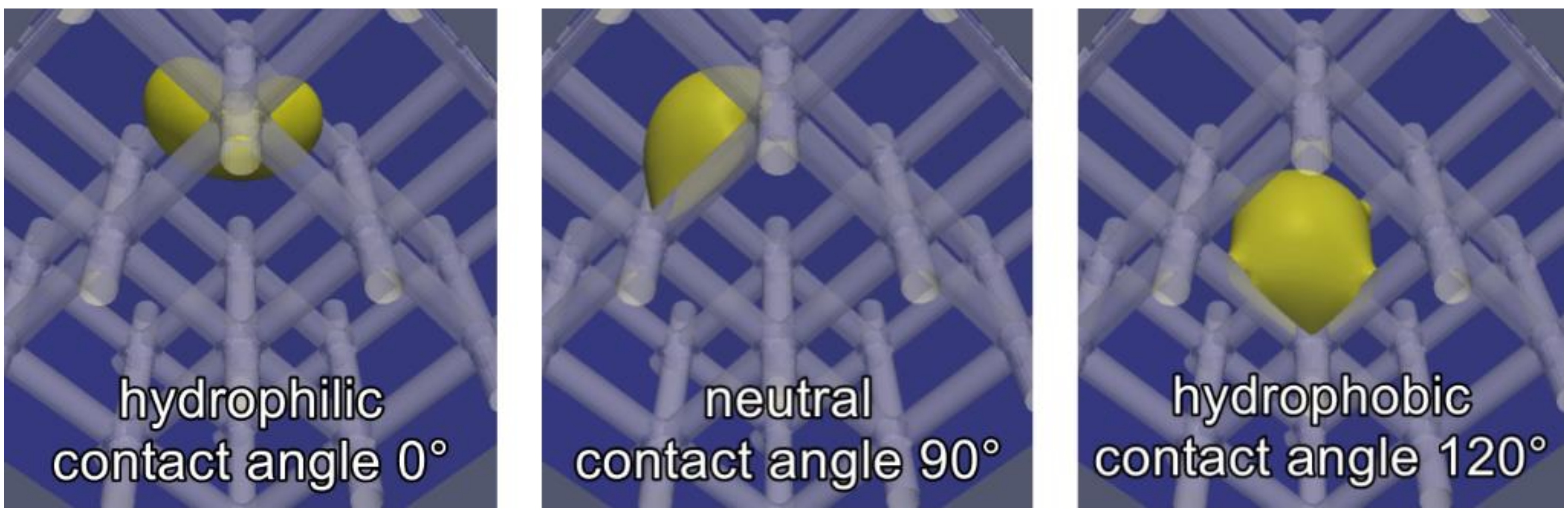
9th International Conference on Multiphase Flow, Firenze (Italy), May 22-27, 2016

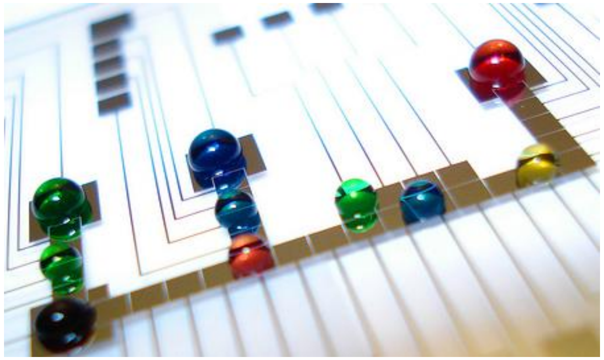


Outline

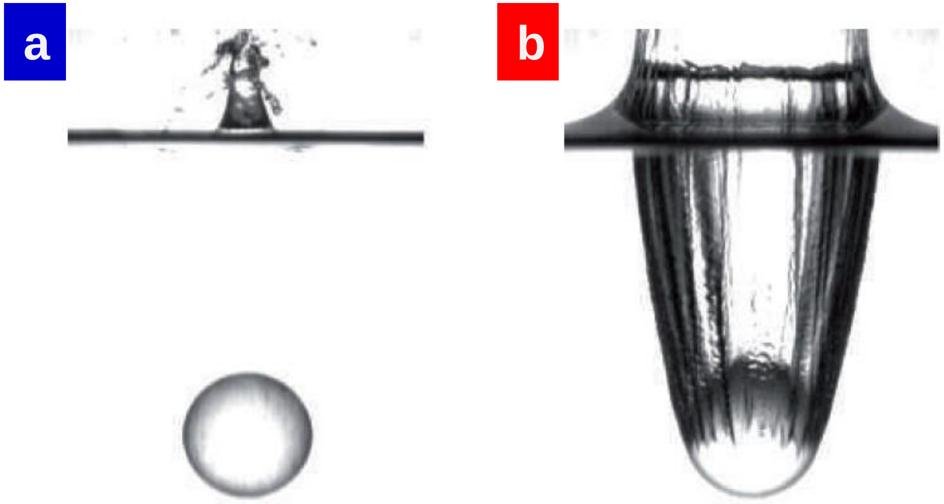
- Motivation
- Numerical method
  - Phase-field method
  - Implementation in OpenFOAM
  - Droplet applications and validation
- Bubble interaction with solid structures
  - Bubble-cutting by a solid cylinder (validation)
  - Influence of cylinder wettability
  - Bubble rise through a periodic open cellular structure (POCS)
- Summary

Motivation

- Manufacturing techniques allow adjustment of **wettability properties** of solid surfaces (static contact angle θ_e) through roughness (lotus effect) or chemical patterning
  - lab-on-a-chip systems
  - drag reduction
  - …
- Wettability can have dramatic effect on macroscopic hydrodynamics



http://www.chemistry-blog.com/2010/06/26/art-on-a-chip/



Impact of two spheres differing only in wettability via a nanometric coating on their surface

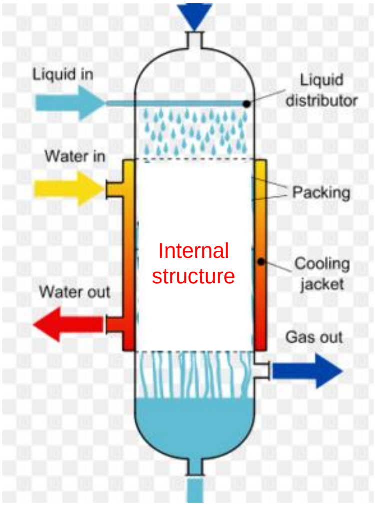
a hydrophilic, θ_e =15°

b hydrophobic, θ_e =100°

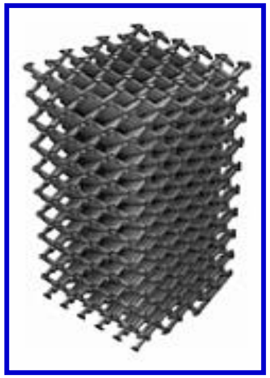
Duez et al., *Nature Physics* **3** (2007) 180-183

Motivation (continued)

- Additive manufacturing allows fabrication of complex solid structures
  - Example: internals for multiphase chemical reactors (e.g. bubble columns)



Multiphase chemical reactor with structured packing



Solid sponge (see presentation of X. Cai in session "Interfacial Flows", Tu 16:20-17:40, Room: Affari-2.A)

Periodic Open Cellular Structure (POCS) manufactured at FAU Erlangen-Nürnberg

***Question:* how should the POCS wettability be designed to enhance mass transfer and reaction?**

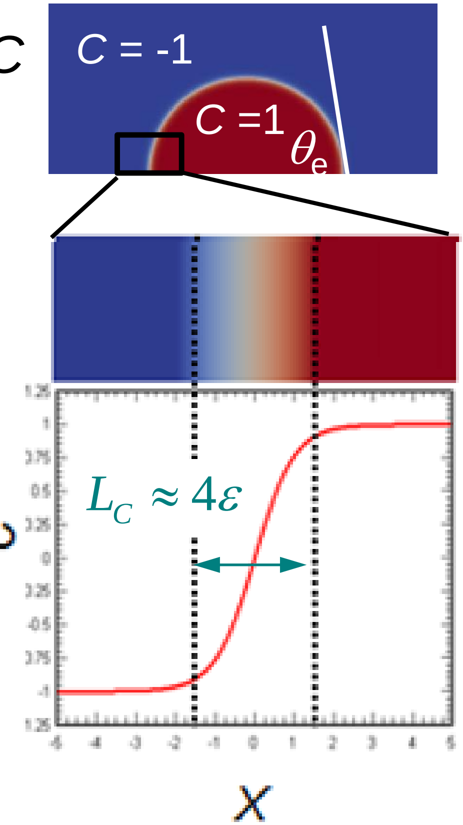
- Goal: Study wettability dependent interaction of gas-liquid flows with solid structures by "direct" numerical simulation
- Method of choice: **phase-field (PF) method**
  - Do-Quang & Amberg (2009) simulated exp. of Duez using a PF method

📖 M. Do-Quang, G. Amberg, *Phys. Fluids* **21** (2009) 022102

Phase field method

- Phase distribution is described by order parameter C
- Diffuse interface representation
  - Smooth transition layer between phases
  - Thickness is characterized by capillary width $\varepsilon > 0$
  - 1D equilibrium profile $C(x) = \tanh\left(x/(\sqrt{2}\varepsilon)\right)$
- Evolution of C by convective Cahn-Hilliard equation

$$\boxed{\frac{\partial C}{\partial t} + (\mathbf{u} \cdot \nabla) C = \kappa \nabla^2 \phi(C)} \qquad \phi = \frac{\lambda}{\varepsilon^2} C(C^2 - 1) - \lambda \nabla^2 C$$



  - ϕ = chemical potential [J/m³]
  - λ = mixing energy parameter [J/m]
  - κ = mobility [m³s/kg]
- Wetting boundary condition $\hat{\mathbf{n}}_s \cdot \nabla C = \frac{\sqrt{2}}{2} \frac{\cos\theta_e}{\varepsilon}(1 - C^2)$
  - θ_e = equilibrium contact angle
  - Diffusive mechanism for contact line motion at a no slip wall $\frac{\partial C}{\partial t} = \kappa \nabla^2 \phi(C)$

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

Coupling with momentum equation

- Navier-Stokes equation for two incompressible Newtonian fluids

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

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

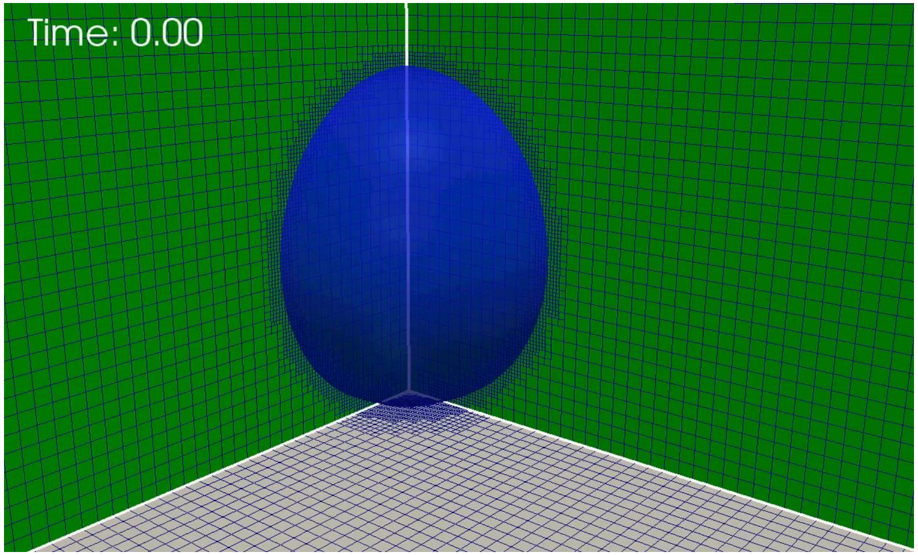
$$\rho_C = \frac{1+C}{2}\rho_{\mathrm{L}} + \frac{1-C}{2}\rho_{\mathrm{G}}, \quad \mu_C = \frac{1+C}{2}\mu_{\mathrm{L}} + \frac{1-C}{2}\mu_{\mathrm{G}}, \quad \mathbf{f}_\sigma = -C\nabla\phi$$

- Fixing the PF method specific parameters ε, λ, κ
  - Cahn number $Cn = \varepsilon / L$
    - L = characteristic macroscopic length scale (here bubble diameter)
  - Mobility based Peclet number $Pe_C = \sqrt{8/9} L U \varepsilon / (\kappa \sigma)$
    - U = characteristic velocity scale (here $U = \sigma / \mu_{\mathrm{L}}$)
  - Coefficient of surface tension $\sigma = 2\sqrt{2}\lambda / (3\varepsilon)$

📖 D. Jacqmin, *J. Comput. Phys.* **155** (1999) 96-127; J. Kim, *Commun. Comput. Phys.* **12** (2012) 613-661

Implementation in OpenFOAM®

- The method is implemented in OpenFOAM (foam-extend-1.6 and 3.2) as a novel top-level OpenFOAM® solver **phaseFieldFoam**
- Details of numerical method will be published in Marschall et al. (2016)
  - Approximation of spatial derivatives by high-resolution scheme (Gauss Gamma)
  - Time integration by a 2nd order two-time-level backward scheme (Gear's method)
  - Relative density flux term in momentum equation for better volume conservation at high density ratios (similar to Ding et al. and Abels et al.)



$\theta_e = 60°$

📖 H. Marschall et al. (2016), in preparation

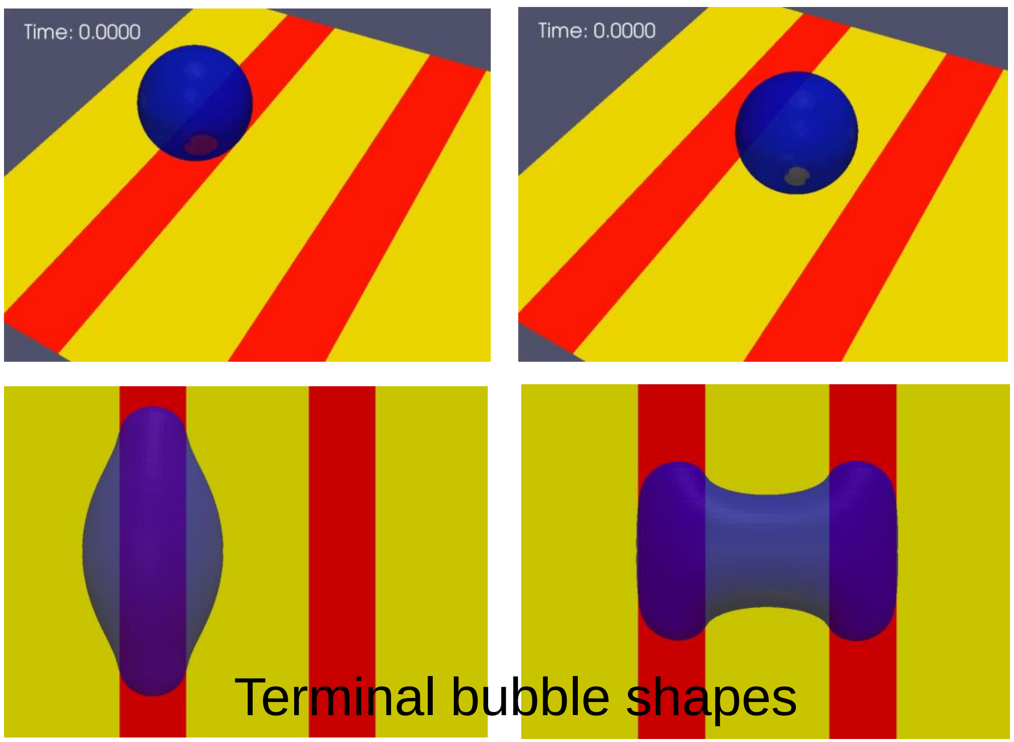
📖 H. Ding et al., *J. Comput. Phys*. **226** (2007) 2078-2095; H. Abels et al., *Math. Mod. Meth. Appl. S*. **22** (2012) 1150013

Validation of phaseFieldFoam

- Comprehensive validation for test problems with analytical solution
  - 🕮 X. Cai et al., *Chem. Eng. Technol.* **38** (2015) 1985–1992
- **Spreading of a droplet on a chemically patterned substrate**
  - Experiments by Léopoldès et al. (inkjet droplets with radius 11µm)
  - PhaseFieldFoam simulations by S. Yadav

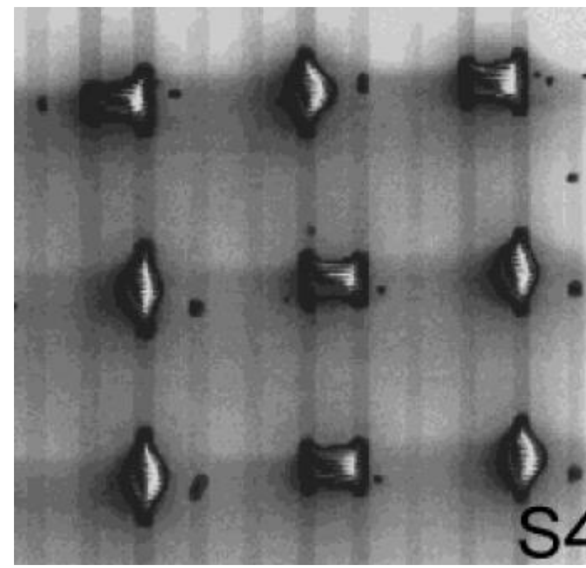
$\theta_e = 20°$

$\theta_e = 64°$



Terminal bubble shapes

$\theta_e = 5°$ $\theta_e = 64°$

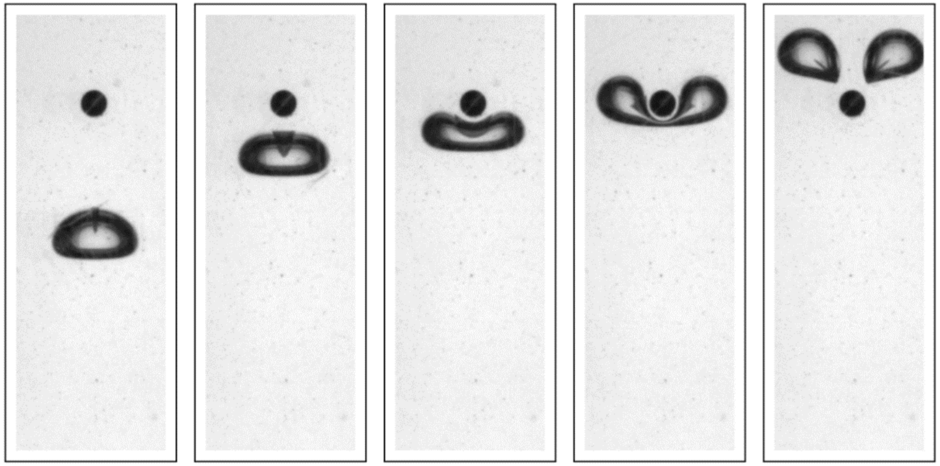


Terminal experimental droplet shapes
🕮 Léopoldès et al. *Langmuir*, 19 (2003) 9818–9822

Bubble-cutting experiment of Segers

(group of Hans Kuipers)

- Air bubble rising in liquid glycerin
  - Variation of bubble diameter (Eötvös number) $Eo = (\rho_L - \rho_G) g D_B^2 / \sigma$
  - Variation of liquid viscosity (Morton number) $Mo = (\rho_L - \rho_G) g \mu_L^4 / (\rho_L^2 \sigma^3)$
  - Head-on and oblique collision between bubble and cylinder



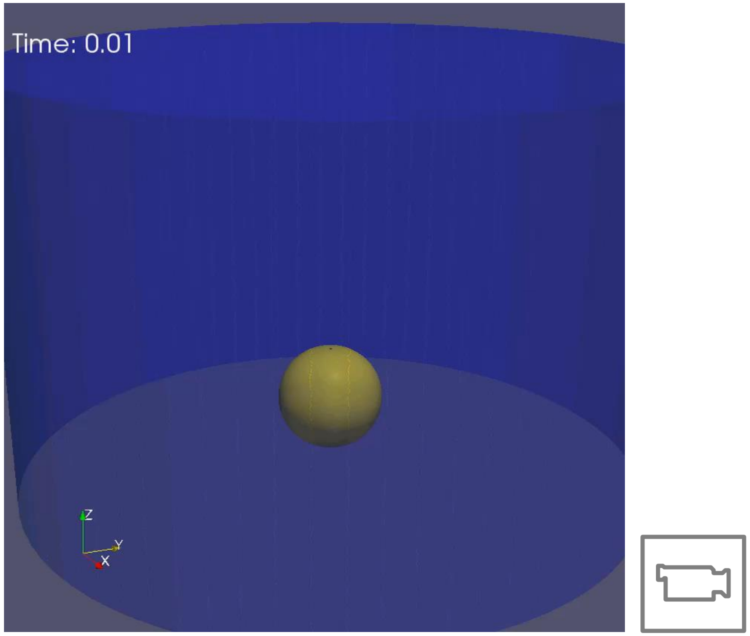
- Parameters and fluid properties for present simulations
  - Only head-on collisions
  - Morton number *Mo* = 0.064

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

Procedure

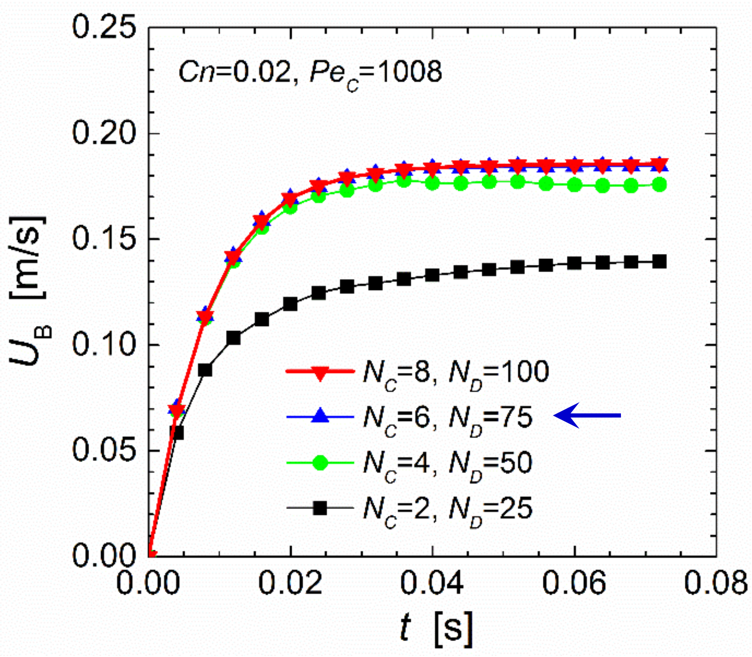
- Validate for terminal bubble rise velocity
- Validate for instantaneous bubble cutting process
- Study influence of wettability on bubble cutting process

2D axisymmetric simulations
Uniform grid with mesh size *h*



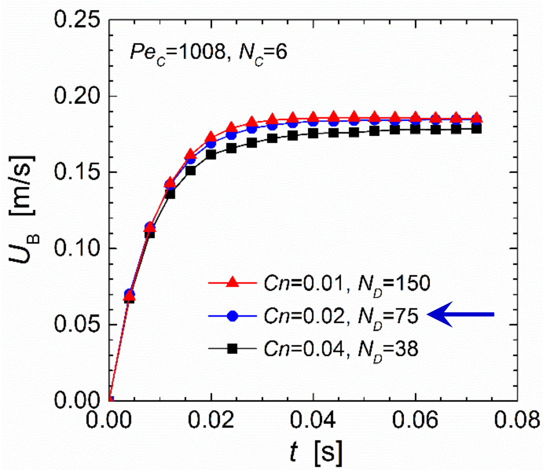
Influence of mesh resolution

$$N_C = \frac{L_C}{h} = \frac{4\varepsilon}{h} \qquad N_D = \frac{D_B}{h} = \frac{N_C}{4Cn}$$

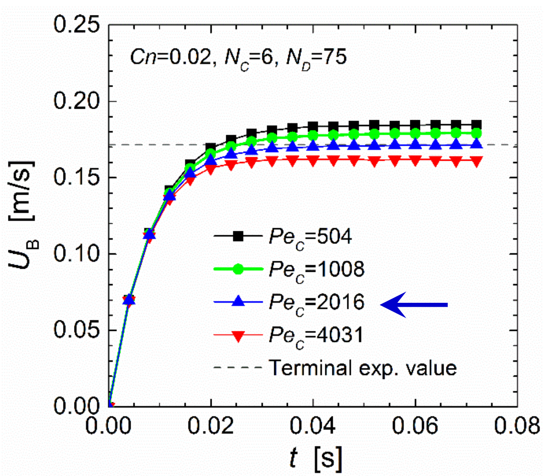


Terminal bubble rise velocity

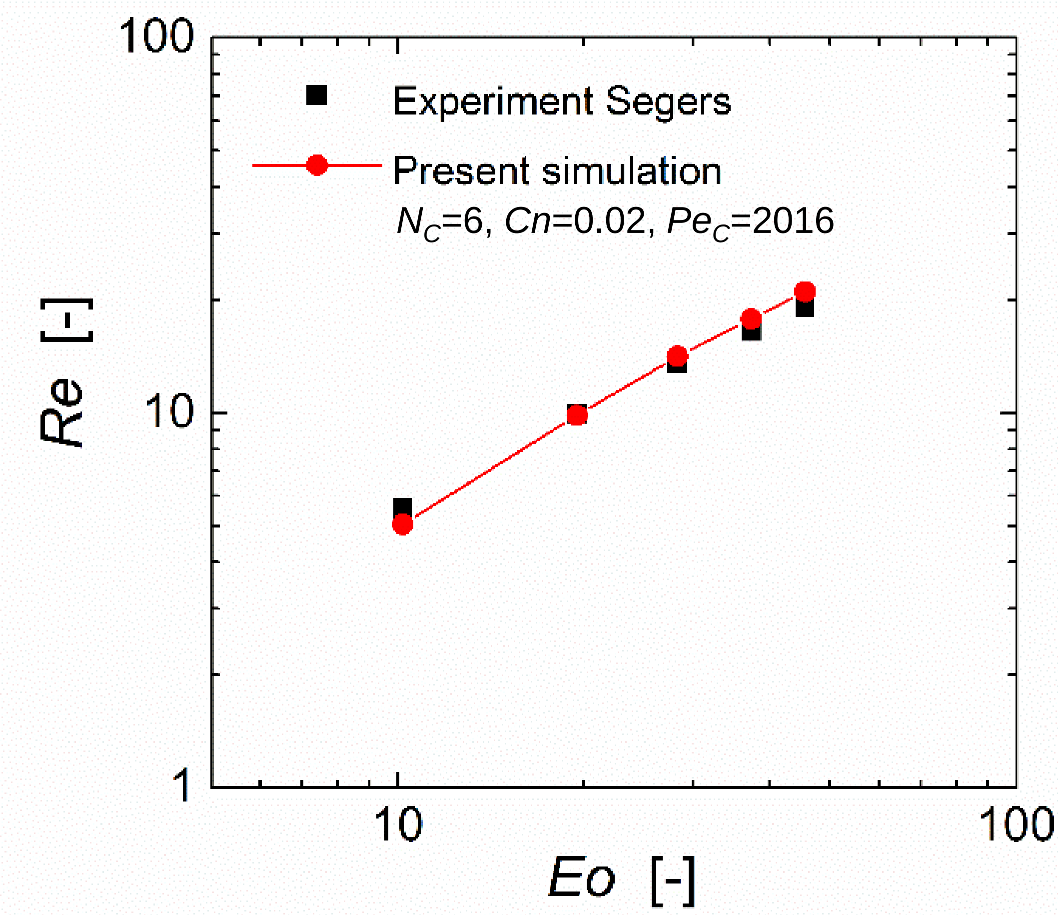
Influence of Cahn number



Influence of Peclet number



Comparison with experiment

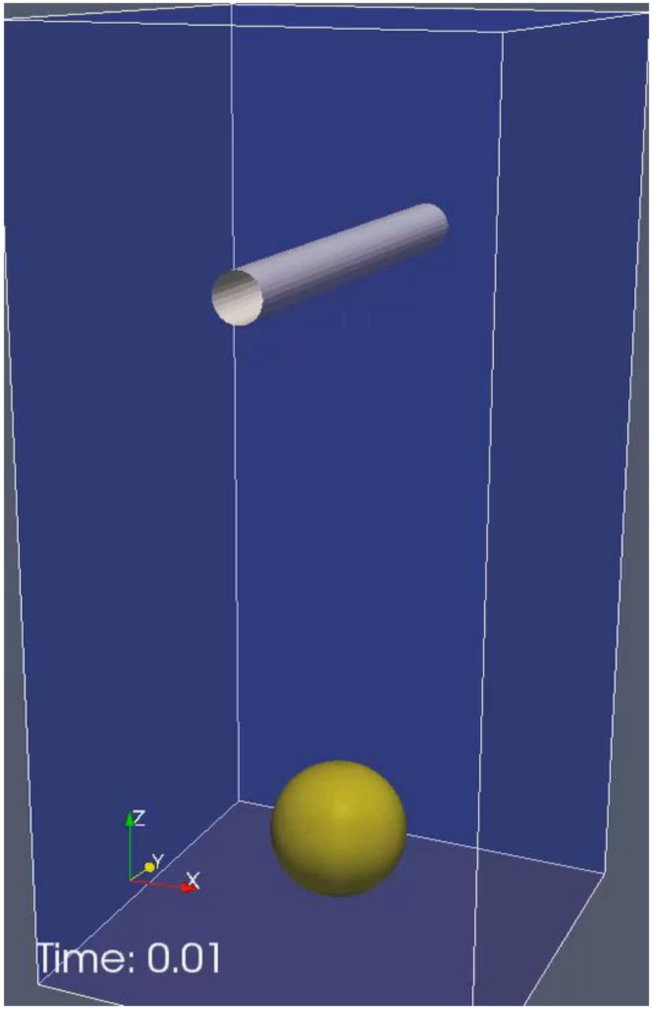


Cylinder-induced bubble break up

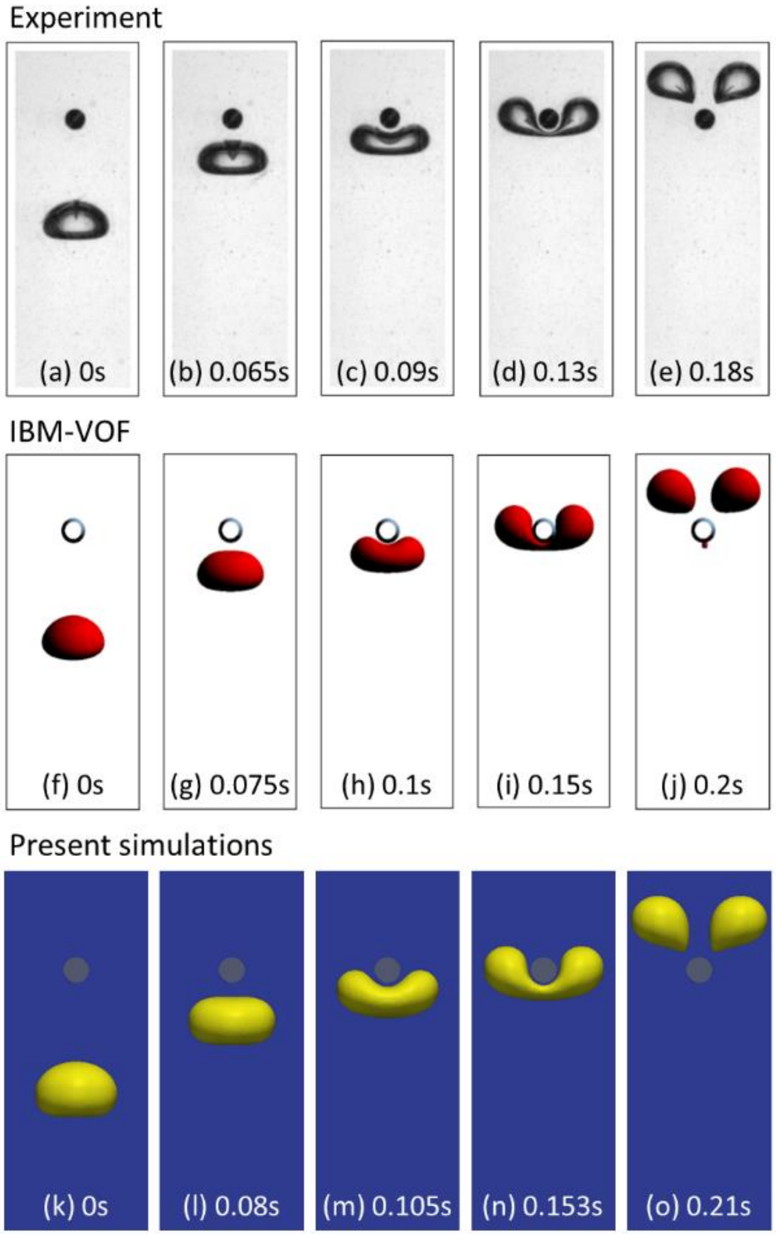
- Parameters according exp. of Segers
  - Bubble diameter D_B = 9.1 mm
  - Diameter of solid cylinder D_{cyl} = 3.1 mm
  - Cylinder is made of stainless steel
  - Contact angle θ_e was not measured, is estimated to be about 60°
- Simulation set-up
  - 3D simulation, one quarter with symmetry boundary conditions
  - Cross section $2D_B \times 2D_B$, height $6D_B$
  - $N_C = 4$
  - $Cn = 0.04$
  - $Pe_C = 1000$

$$N_{\text{cells}} \propto \left(\frac{N_C}{Cn}\right)^3$$

$\theta_e = 60°$



📖 X. Cai, M. Wörner, H. Marschall and O. Deutschmann, *Catalysis Today*, **2016**, in press (available online)



Experiment Segers

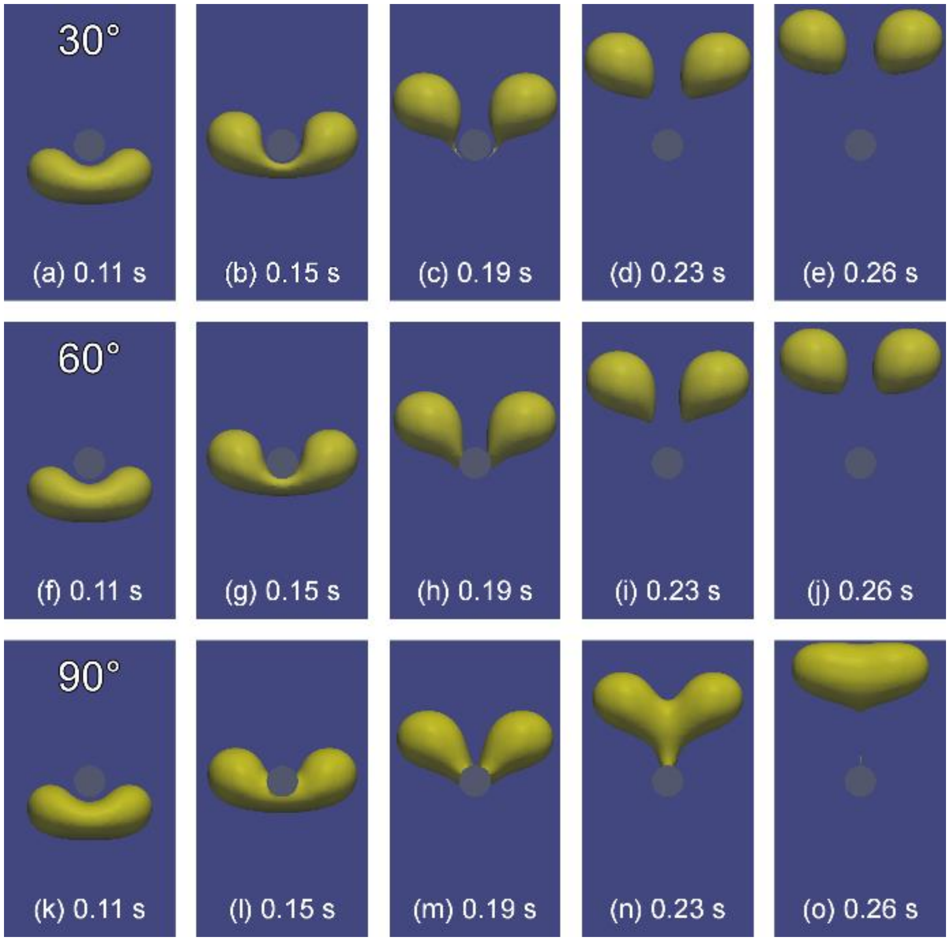
Numerical simulation of Segers with IBM-VOF method, see also

📖 Baltussen et al., Cutting bubbles with a single wire, *Chem. Eng. Sci.*, in press

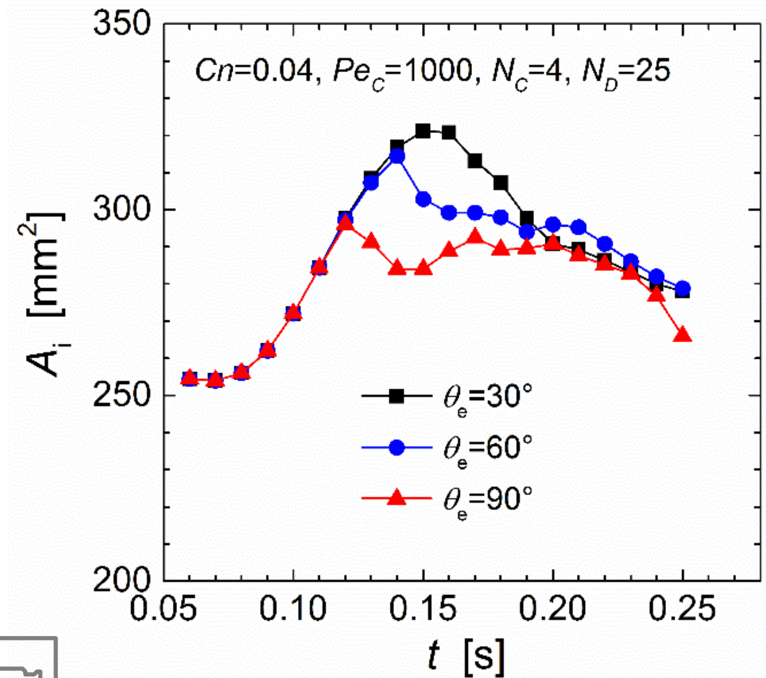
Present phase field simulation
$\theta_e = 60°$

← *Time in figures is slightly different*

Influence of cylinder wettability



Gas-liquid interfacial area A_i



Periodic Open Cellular Structures

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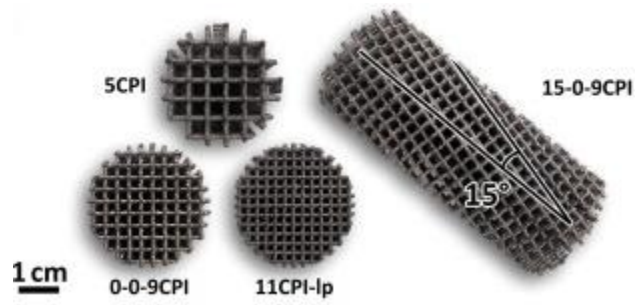
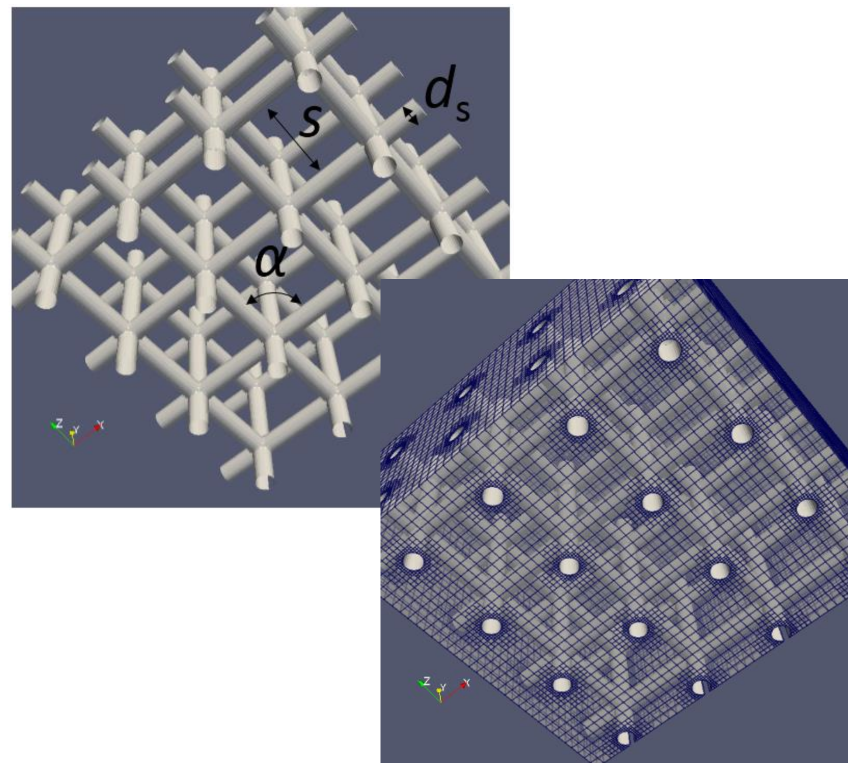
- POCS of different geometry are manufactured at FAU Erlangen-Nürnberg (e.g. by SEBM)
  - Here a POCS with cubic cell geometry is considered
- Geometric parameters
  - Window size s = 4 mm
  - Strut diameter d_s = 1 mm
  - Grid angle α = 90°
  - Entire POCS is titled by 45°
  - STL geometry for mesh generation provided by C.O. Möller, TUHH
- Simulation parameters
  - Air bubble in water (stagnant)
  - Bubble diameter D_B = 4 mm
  - Locally refined static mesh

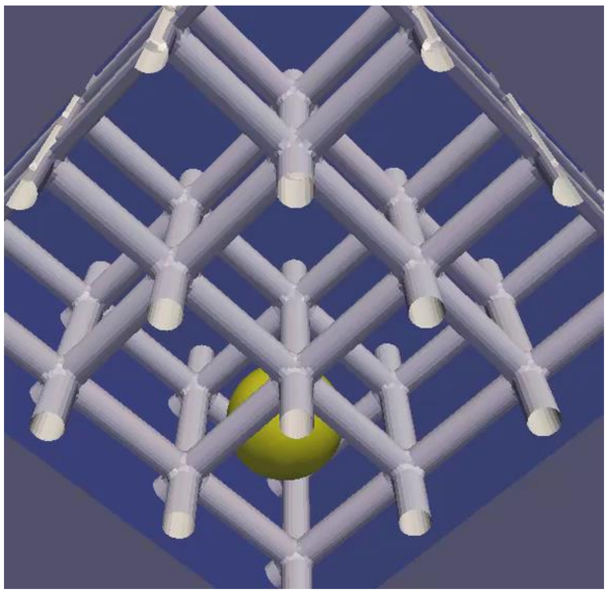


📖 M. Klumpp et al., *Chem. Eng. J.*, **242** (2014) 364-378

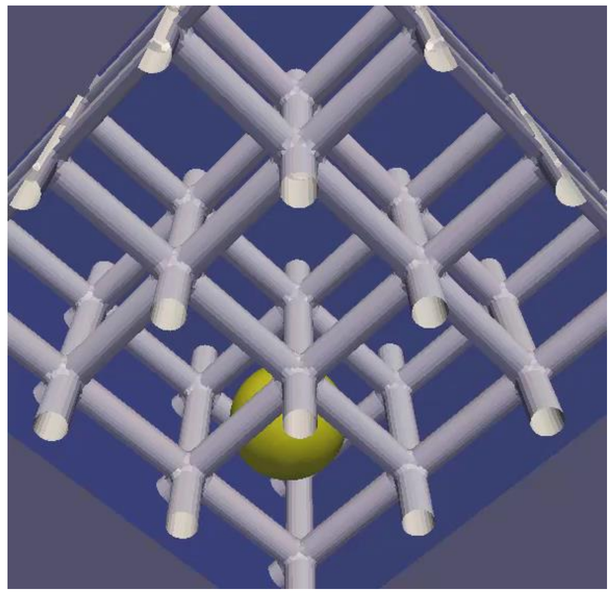


Bubble rise (perspective view)

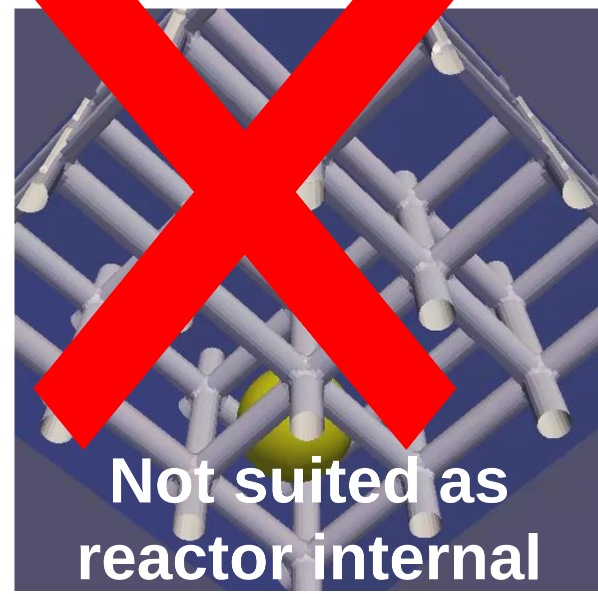
$\theta_e = 0°$
(hydrophilic)



$\theta_e = 90°$



$\theta_e = 120°$
(hydrophobic)



Decreasing wettability (increasing contact angle)

Bubble rise (lateral view)

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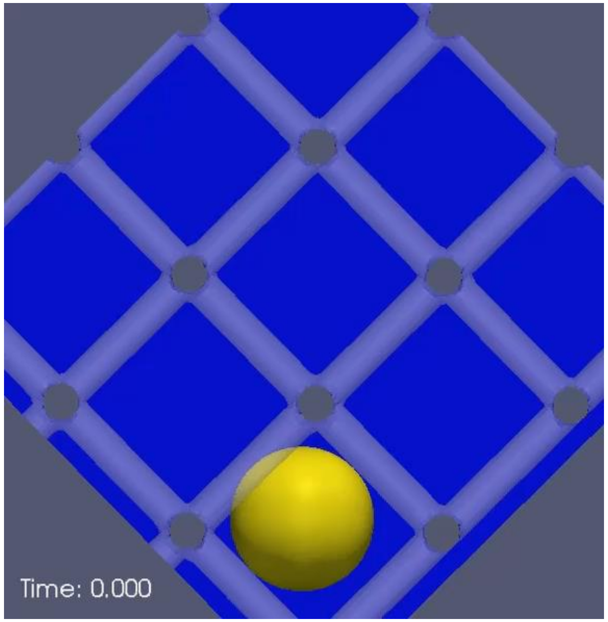
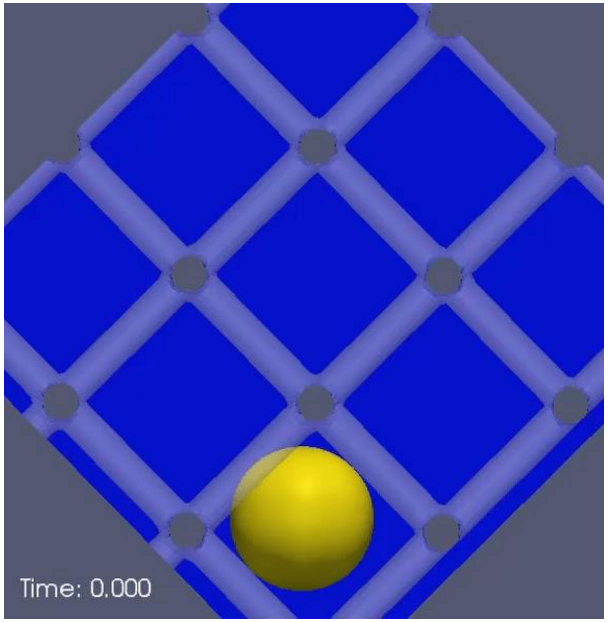
$\theta_e = 0°$



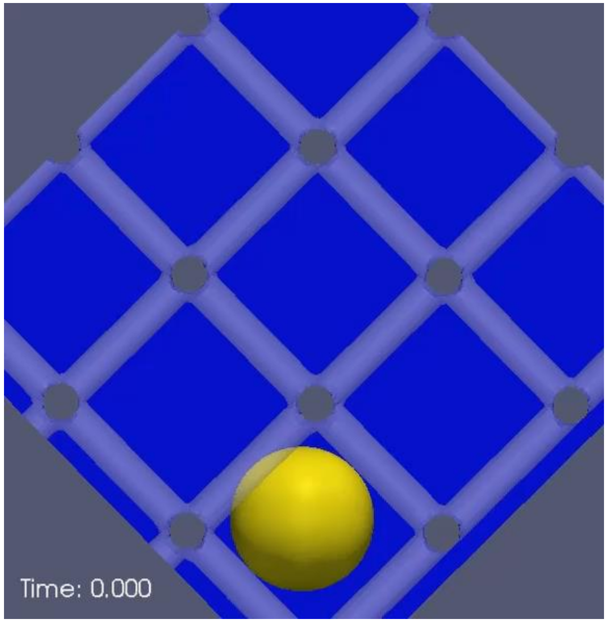
- Bubble is not in contact with struts

$\theta_e = 60°$



- Bubble is in (slight) contact with struts

$\theta_e = 90°$



- Bubble is in strong contact with struts and climbs them up

Conclusions

- Implementation of phase-field method coupled with Navier-Stokes equations in OpenFOAM® (*phaseFieldFoam*)
  - Method can well describe wetting phenomena **+**
  - Method can handle real density and viscosity ratios **+**
  - Difficulty to choose appropriate value for mobility parameter **-**
  - *Methods globally conserves C but not bubble volume* **-**
- The numerical results for the cylinder-induced bubble cutting and bubble rise in POCS indicate that the bubble shape and path do significantly depend on the structure wettability
- In industrial application of POCS for enhancing mass transfer and as catalytic support structures with high wettability are expected to be beneficial

Acknowledgements

- Funding by Helmholtz Association Energy Alliance “Energy-efficient chemical multiphase processes”
- Thanks to project partners from FAU Erlangen-Nürnberg (Prof. Freund, Prof. Schwieger) and TU Hamburg-Harburg (Prof. Schlüter, C.O. Möller)
- Thanks to internship student S. Yadav (IIT Kharagpur)

Tu 16:20-17:40 **Interfacial Flows**

Room: Affari-2.A; Chairperson: Derksen J.

INTERFACE-RESOLVING SIMULATIONS OF GAS-LIQUID FLOWS IN A SOLID SPONGE STRUCTURE

Cai X., Woerner M., Deutschmann O.