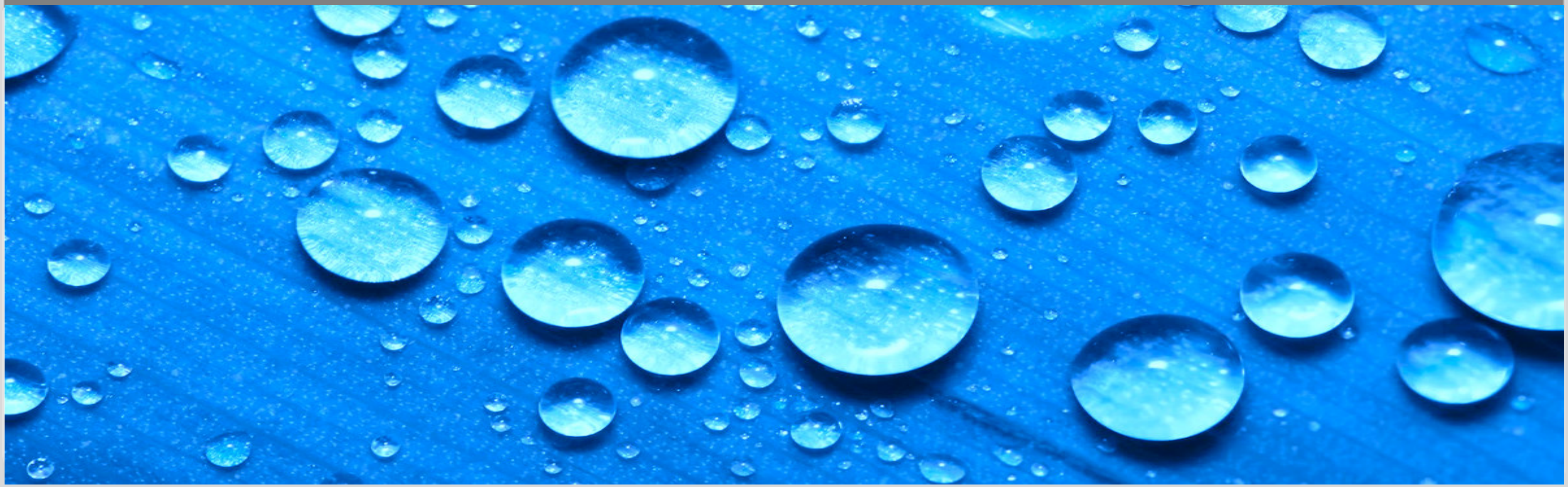
Direct Numerical Simulations for Interface-resolving of Gas-liquid Flows in Solid Sponge Structure

Xuan Cai, Dr. Martin Wörner, Prof. Olaf Deutschmann

Karlsruhe Institute of Technology (KIT), Germany

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

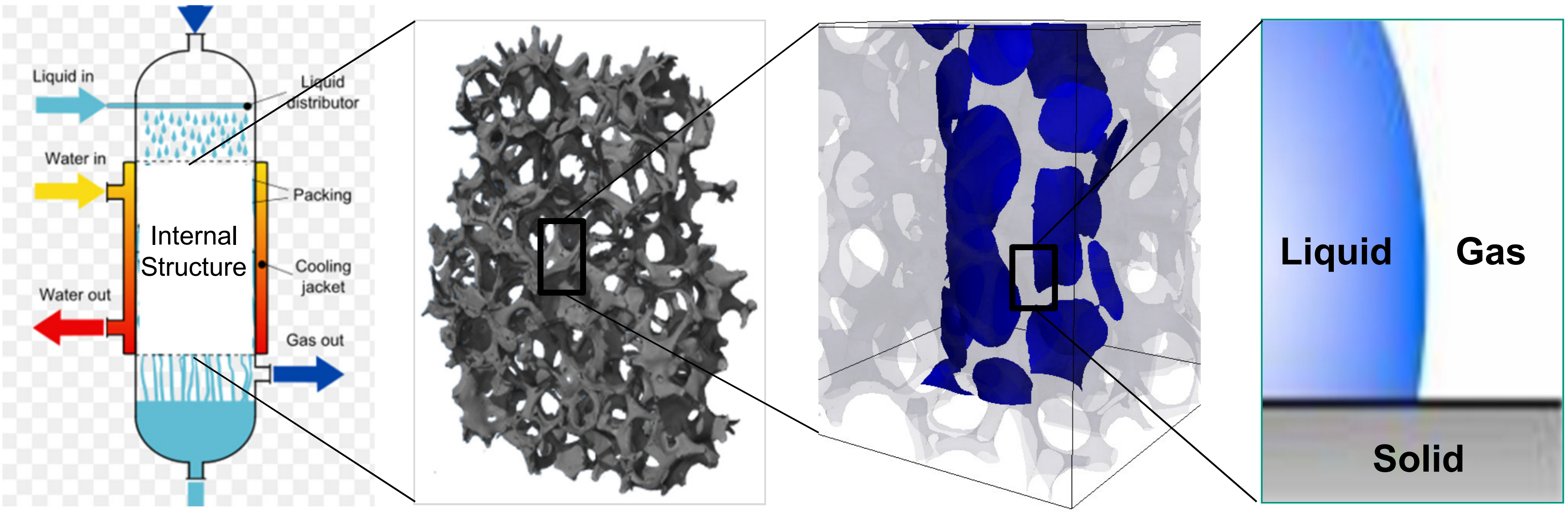


Outline

- Motivation of Direct Numerical Simulations (DNS) for interface resolving
- Phase field method and *phaseFieldFoam* in OpenFOAM
  - Validation for droplet or bubble interacting with solid surface
- DNS for interface-resolving of gas-liquid flows in sponge structure
- Summary & outlooks

Motivation

- Direct numerical simulation for understanding hydrodynamic interaction of gas-liquid interfacial flows with solid surface



Multiphase reactor with structured packings

sponge (i.e. foam) structure

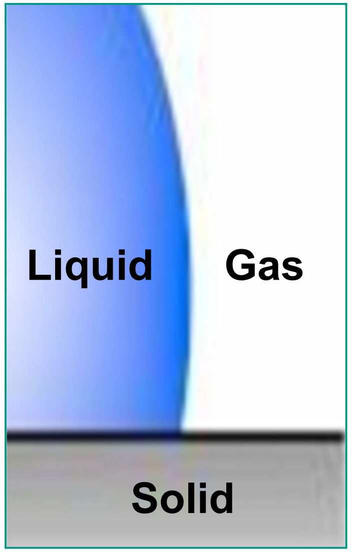
Gas-liquid Interfacial flow in representative domain of sponge structure

dynamics of moving contact line

m **length scale** **µm**

Motivation

- Direct numerical simulation for understanding hydrodynamic interaction of gas-liquid interfacial flows with solid surface



dynamics of
moving contact line

For sharp-interface method, classical paradox between:

- motion of contact line
- no-slip boundary condition

Volume fraction equation in VOF:

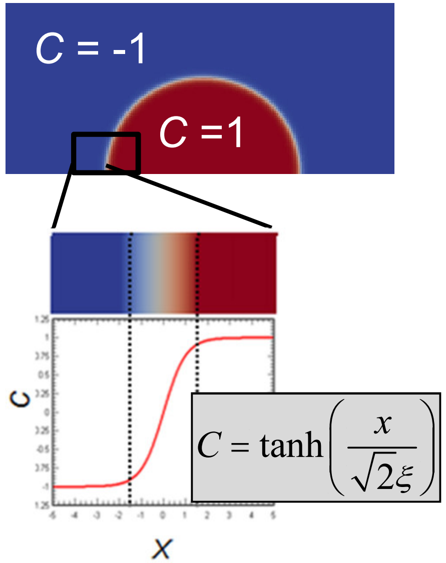
$$\frac{\partial F}{\partial t} + (\mathbf{u} \cdot \nabla) F = 0$$

$\mathbf{u} = 0$ on wall

- Common remedy is to allow for slip at wall by Navier slip BC
- **Another strategy is to abandon “sharp-interface” and embrace “diffuse-interface” concept**

Phase Field Method

- Phase field (C) as phase indictor
  - Smooth transition from -1 to 1 → **diffuse interface**



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

- Phase field evolution governed by Cahn-Hilliard equation

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

describes motion of contact line!

- Wetting boundary condition for static contact angle $\boldsymbol{\theta_e}$

$$\hat{\mathbf{n}}_s\cdot\nabla C = \frac{\sqrt{2}}{2}\frac{\cos\theta_e}{\varepsilon}(1-C^2)$$

Φ = chemical potential [J/m^3]
λ = mixing energy [J/m]
ε = diffuse interface thickness [m]
κ = mobility [m^{3}s/kg]

- Single-field Navier-Stokes equation:

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

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

Method implementation and verification

- Close cooperation with **Dr. Holger Marschall** (TU Darmstadt, Germany)
- Phase field method implemented in OpenFOAM (foam-extend-1.6 & 3.2)
  - A novel OpenFOAM solver **phaseFieldFoam***
- Verification by extensive test cases against analytical solutions**
- Validation by a series of test case for dynamics of droplet or bubble interacting with solid surfaces, such as …

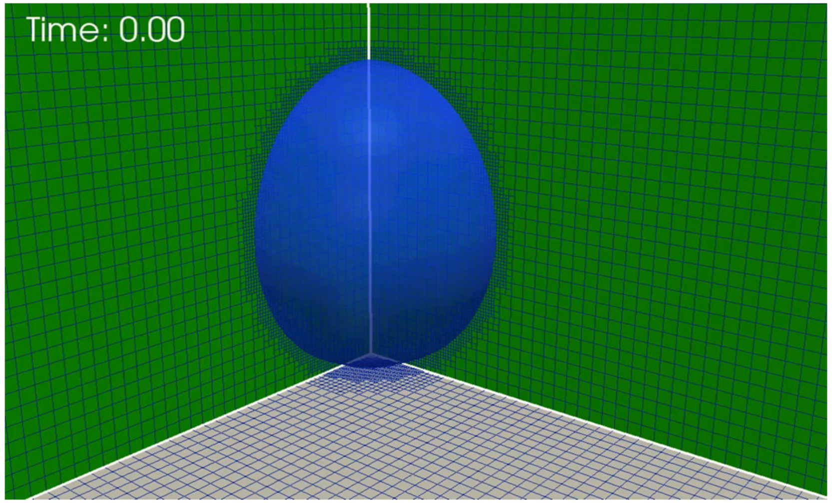
* H. Marschall, X. Cai and M. Wörner. Conservative finite volume discretization of the two-phase Navier Stokes Cahn-Hilliard and Allen-Cahn equations on general grids with applications to dynamic wetting, **2016**, in preparation

** X. Cai, H. Marschall, M. Wörner and O. Deutschmann, *Chem. Eng. Technol.* **2015**, 38: 1985–1992

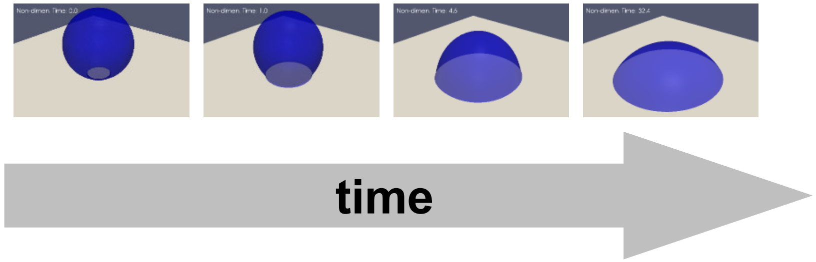
Validation on droplet wetting on flat surface

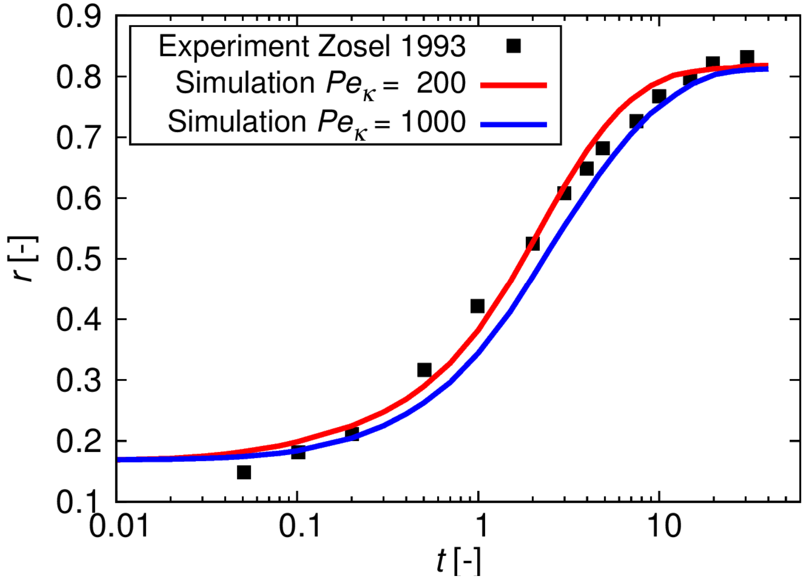
- Experiment by Zosel 1993
  - Diameter ≈ 3 mm
  - PIB solution μ = 25 pa·s
  - smooth PTFE surface (θ_e = 58°)

3D phase-field simulation with
adaptive mesh refinement near interface



Droplet base radius (r) over time



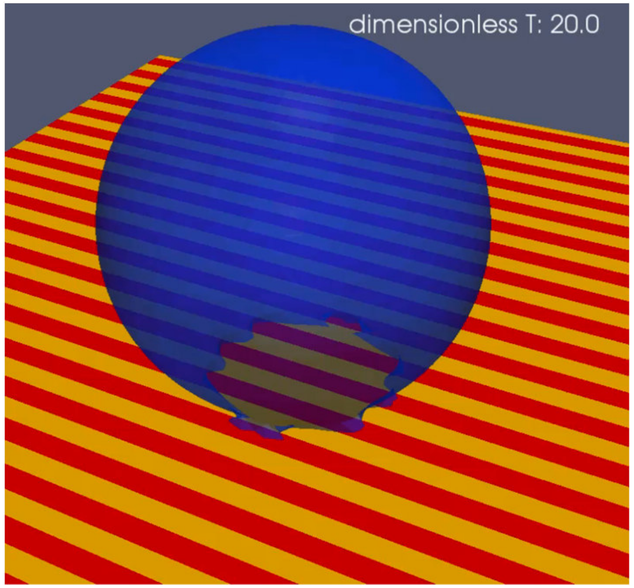


Reference: X. Cai, H. Marschall, M. Wörner and O. Deutschmann, *Chem. Eng. Technol.* **2015**, 38: 1985–1992

Droplet wetting on chemically-patterned surface

- Experiment by Jansen et al. 2013
  - Glycerin droplet volume = 3 μL
  - Alternating stripes made of:

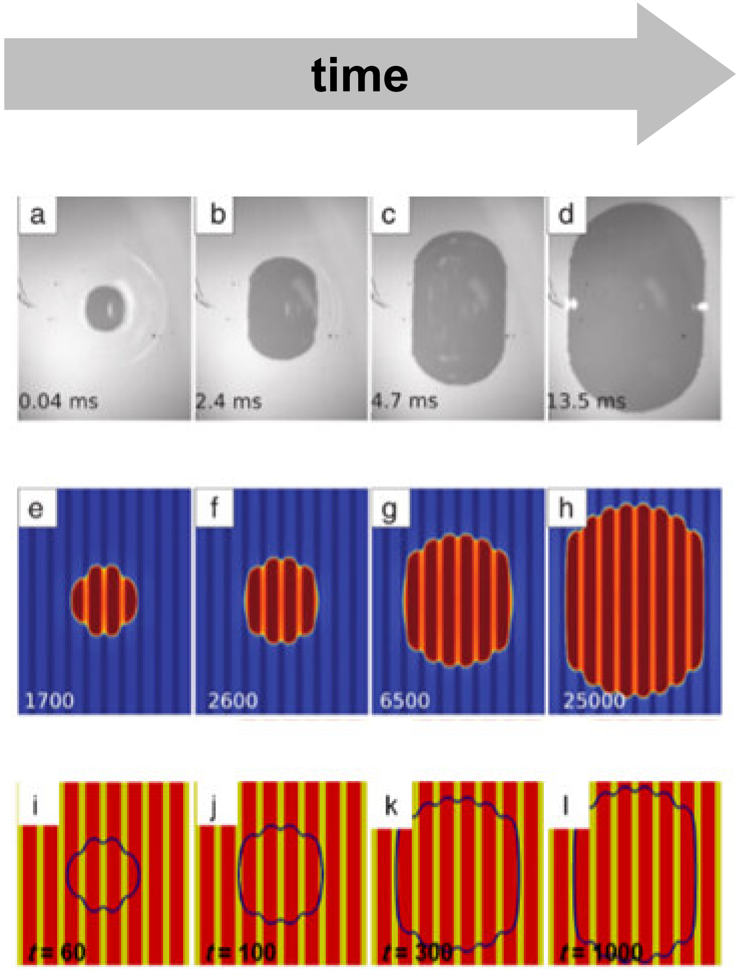
SiO_2,	$\theta_e = 40°$
PFDTS,	$\theta_e = 106°$



Experiment
Jansen et al. 2013

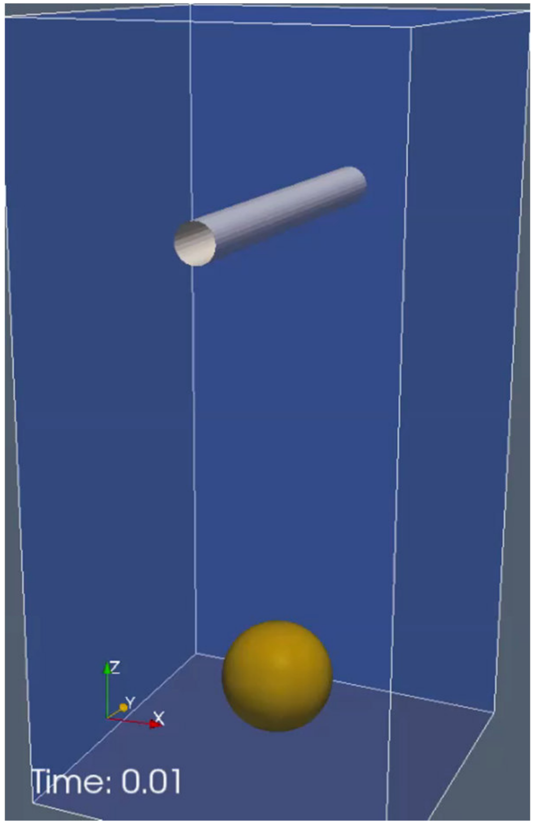
Lattice-Boltzmann Simulation
Jansen et al. 2013

Phase-field Simulation
Cai et al. 2015



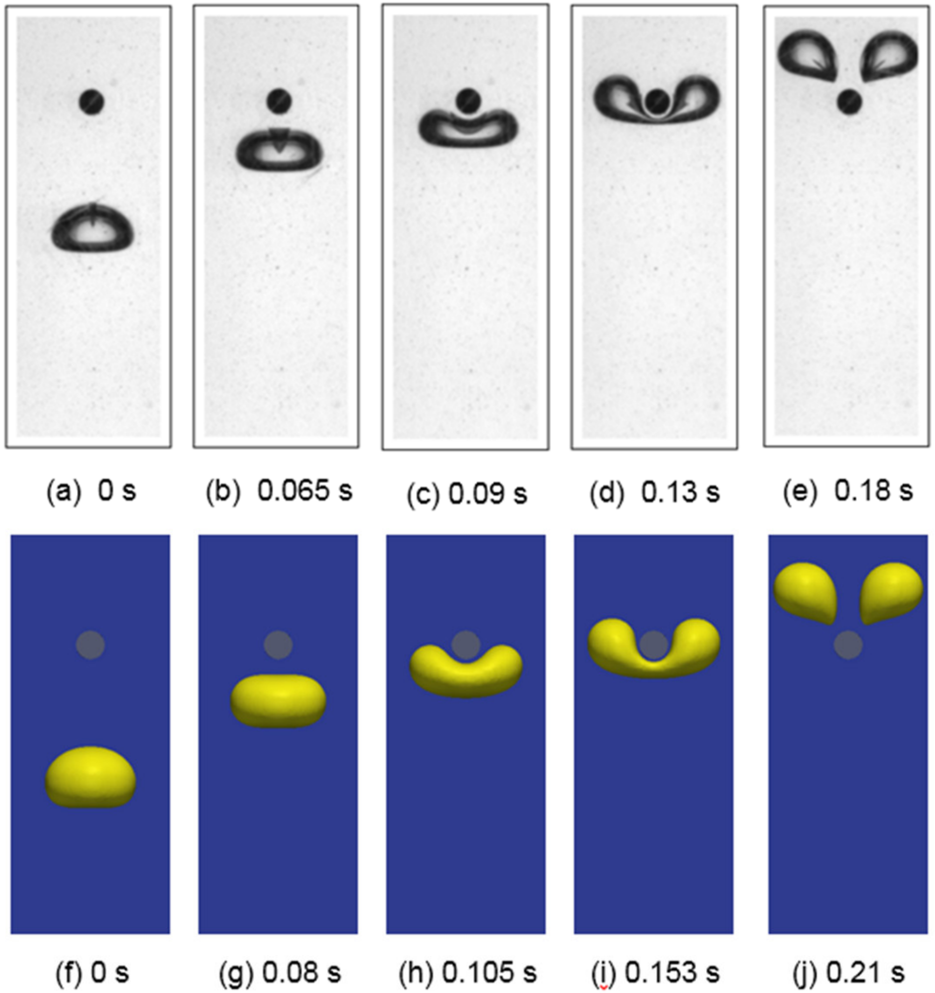
Reference: X. Cai, H. Marschall, M. Wörner and O. Deutschmann, *Chem. Eng. Technol.* **2015**, 38: 1985–1992

Validation on cylinder-induced bubble breakup



Experiment
Segers 2015
(Prof. Kuipers,
Prof. Deen,
TU Eindhoven)

Phase-field
Simulation
Cai et al. 2016



- Diameter of cylinder = 3.1 mm
- Diameter of bubble = 9.1 mm

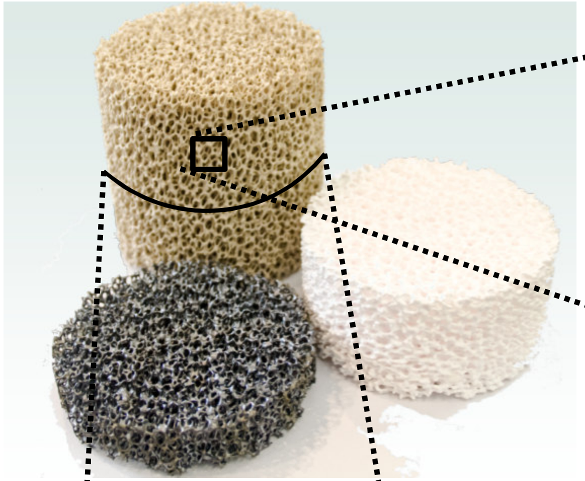
Reference: X. Cai, M. Wörner, H. Marschall and O. Deutschmann, *Catalysis Today*, **2016**, in press

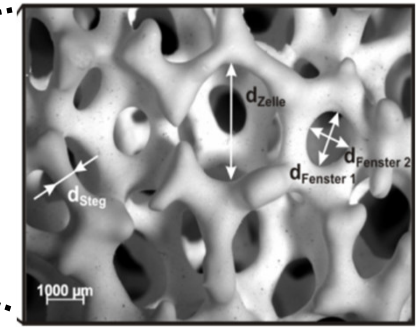
Outline

- Motivation of Direct Numerical Simulations (DNS) for interface resolving
- Phase field method and *phaseFieldFoam* in OpenFOAM
  - Validation for droplet or bubble interacting with solid surface
- DNS for interface-resolving of gas-liquid flows in sponge structure
- Summary & outlooks

Interface-resolving for Two-phase Flow in Sponge

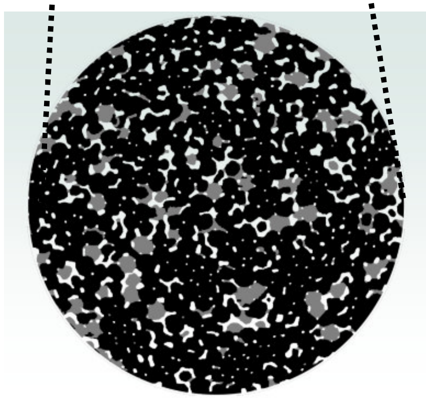
- Total Sponge structure
  - Height: 25 – 100 mm
  - Diameter: 100 mm
- Individual liquid jets
  - Approx. 1 – 10 mm
- Local gas-liquid interface
  - Approx. 0.1 – 1 mm
- **Disparity of length scale up to 10^2 or 10^3!**





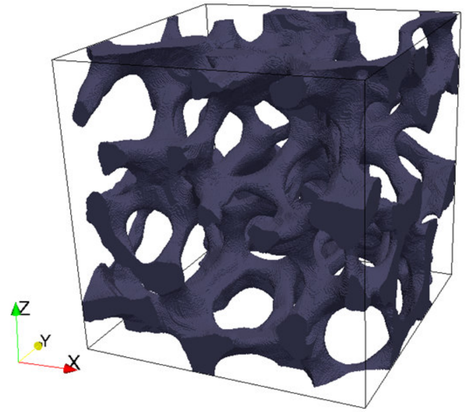
Representative Elementary Volume (REV)

µCT & Reconstruction
S. Meinicke, KIT-TVT



solid
liquid

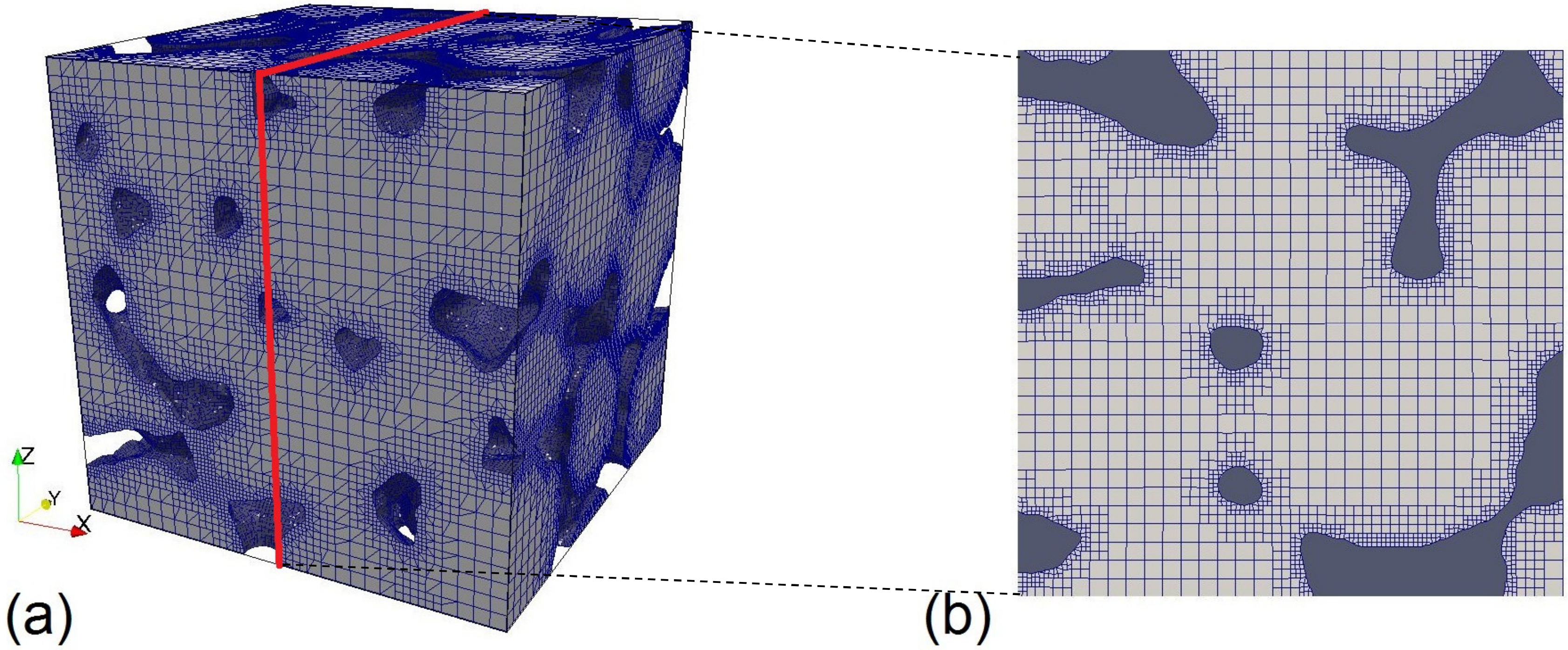
Source: Wallenstein et al. 2015



STL geometry for CFD

Computational mesh for sponge geometry

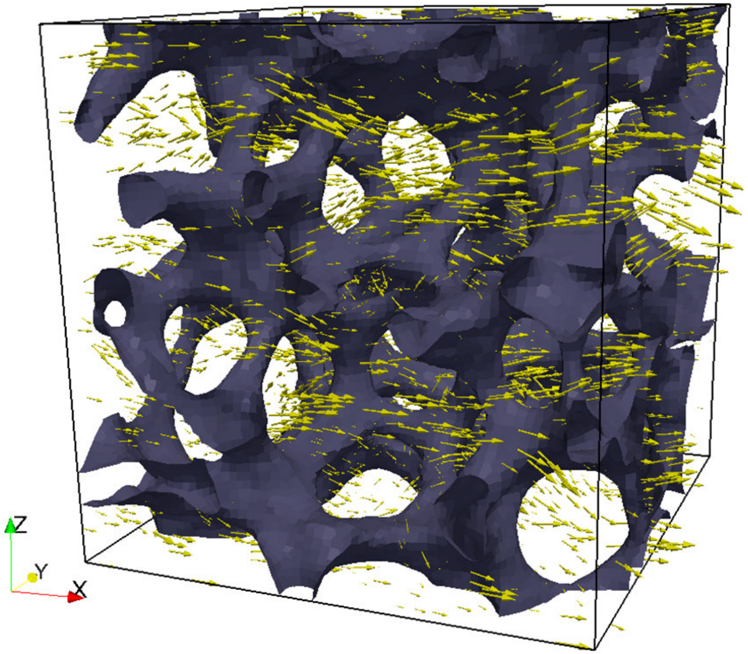
- OpenFOAM's mesh generator *snappyHexMesh*



3D view **2D cross-cutting view**

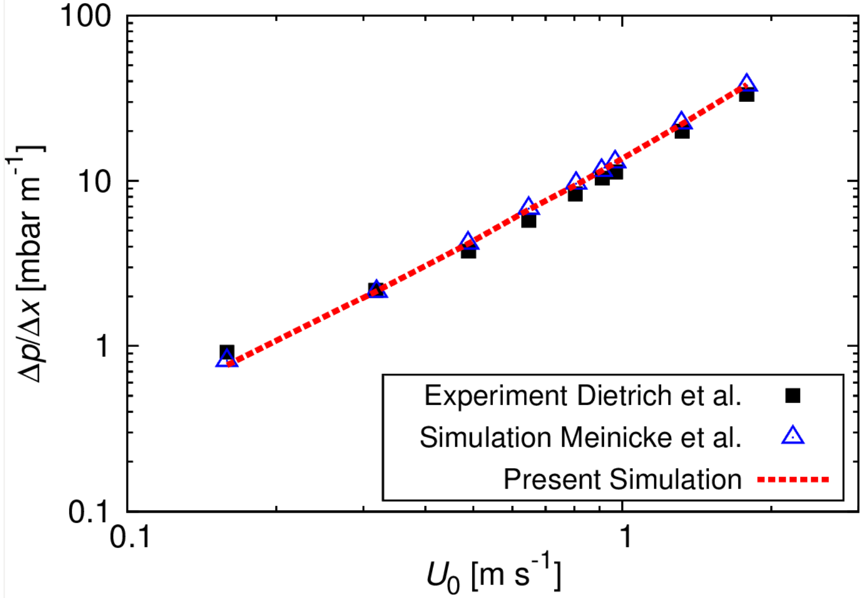
Validation for single-phase gas flow

- Apply the solver for gas flow through sponge structure
  - Compare our simulation results with experiment* and *simpleFoam* simulation**



Gas flow shown by velocity vector (yellow) in a Al_2O_3 sponge, 80% porosity, 20 ppi

pressure drop VS. gas velocity



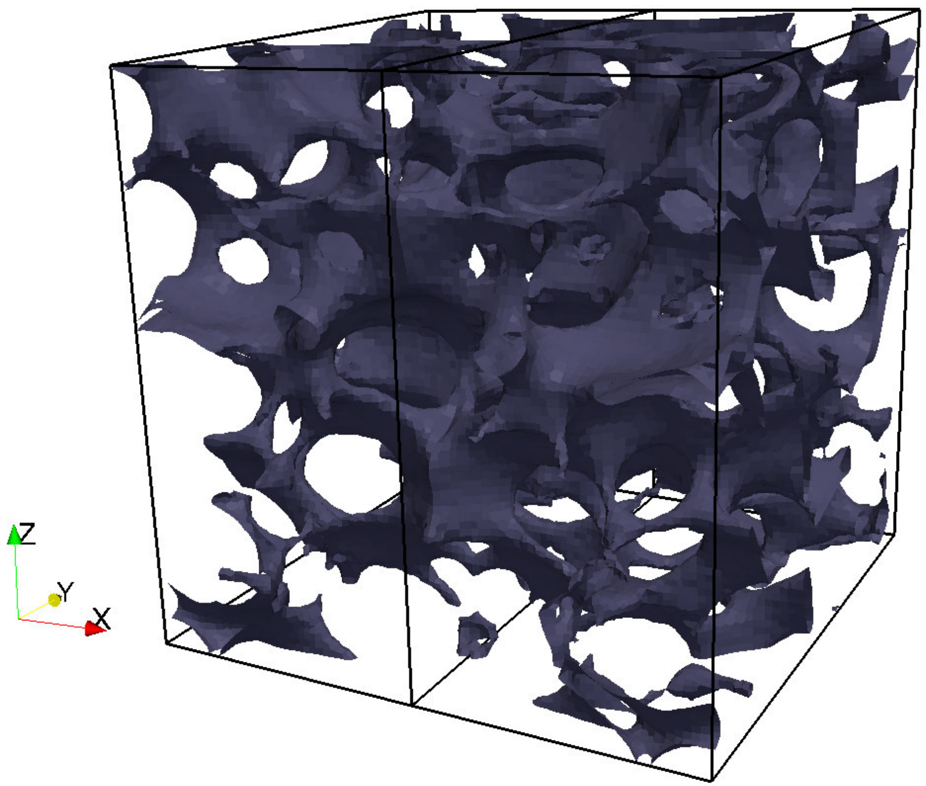
- U_0: superficial gas velocity
- $\Delta p / \Delta x$: pressure drop per unit length

* Dietrich et al. *Chem. Eng. Sci.* 64 (16), 3633-3640. **2009**

** Meinicke et al., *11th Int. Conf. on CFD in the Minerals & Proc. Industries* **2015**

Interface-resolving for Two-phase Flow in Sponge

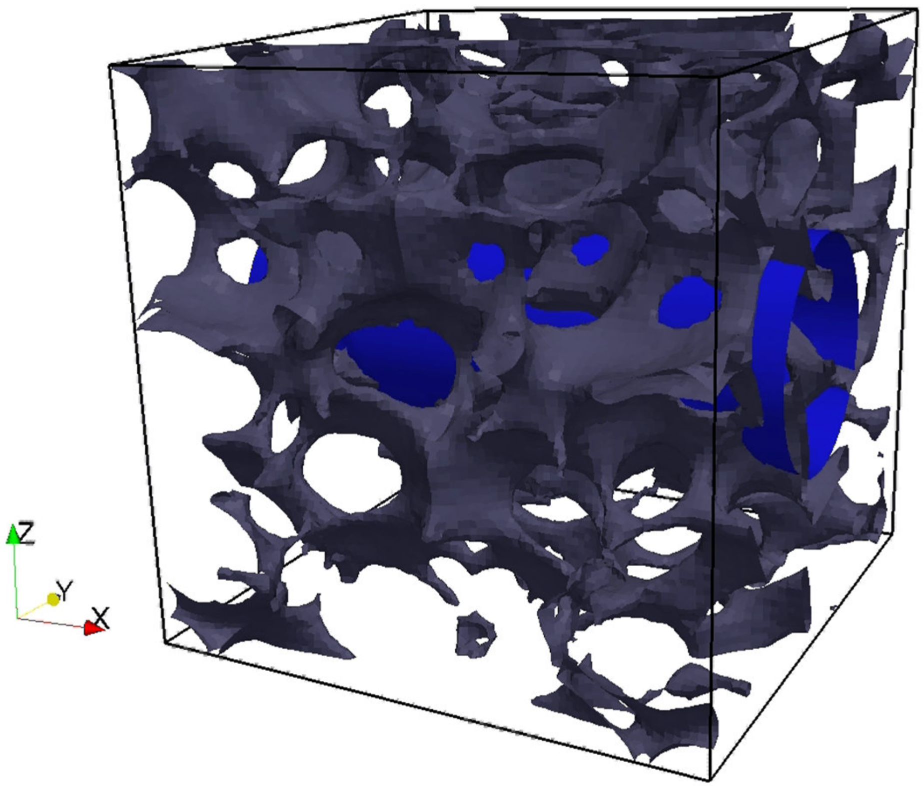
- Representative Elementary Volume → difficult to get inlet liquid distribution from exp.
- Mirroring geometry + periodic boundary conditions



SiSiC foam, 20 ppi, 85% porosity

Interface-resolving for Two-phase Flow in Sponge

- Representative Elementary Volume → difficult to get inlet liquid distribution from exp.
- Mirroring geometry + periodic boundary conditions



SiSiC foam, 20 ppi, 85% porosity

Interface-resolving for Two-phase Flow in Sponge

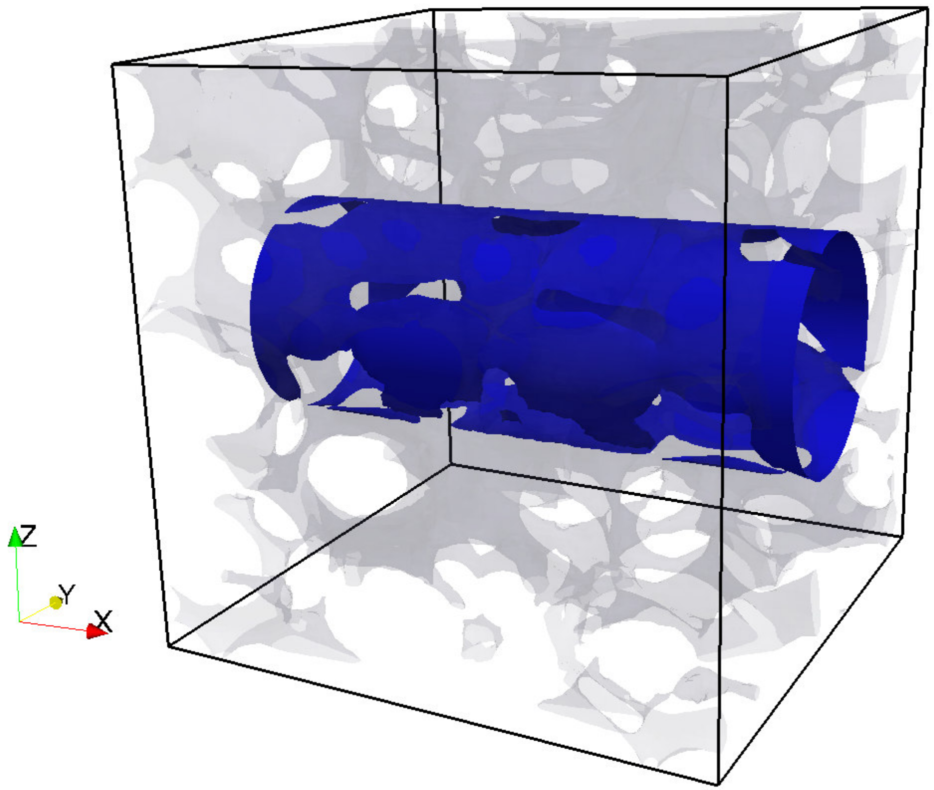
- Conventionally (in experiment): inlet flow rate → pressure drop

- **In current periodic domain: pressure drop → inlet/domain flow rate**

$$p \equiv P - \frac{\overline{p_0} - \overline{p_{L_x}}}{L_x} \cdot \mathbf{x} = P - \mathbf{f}_x \cdot \mathbf{x}$$

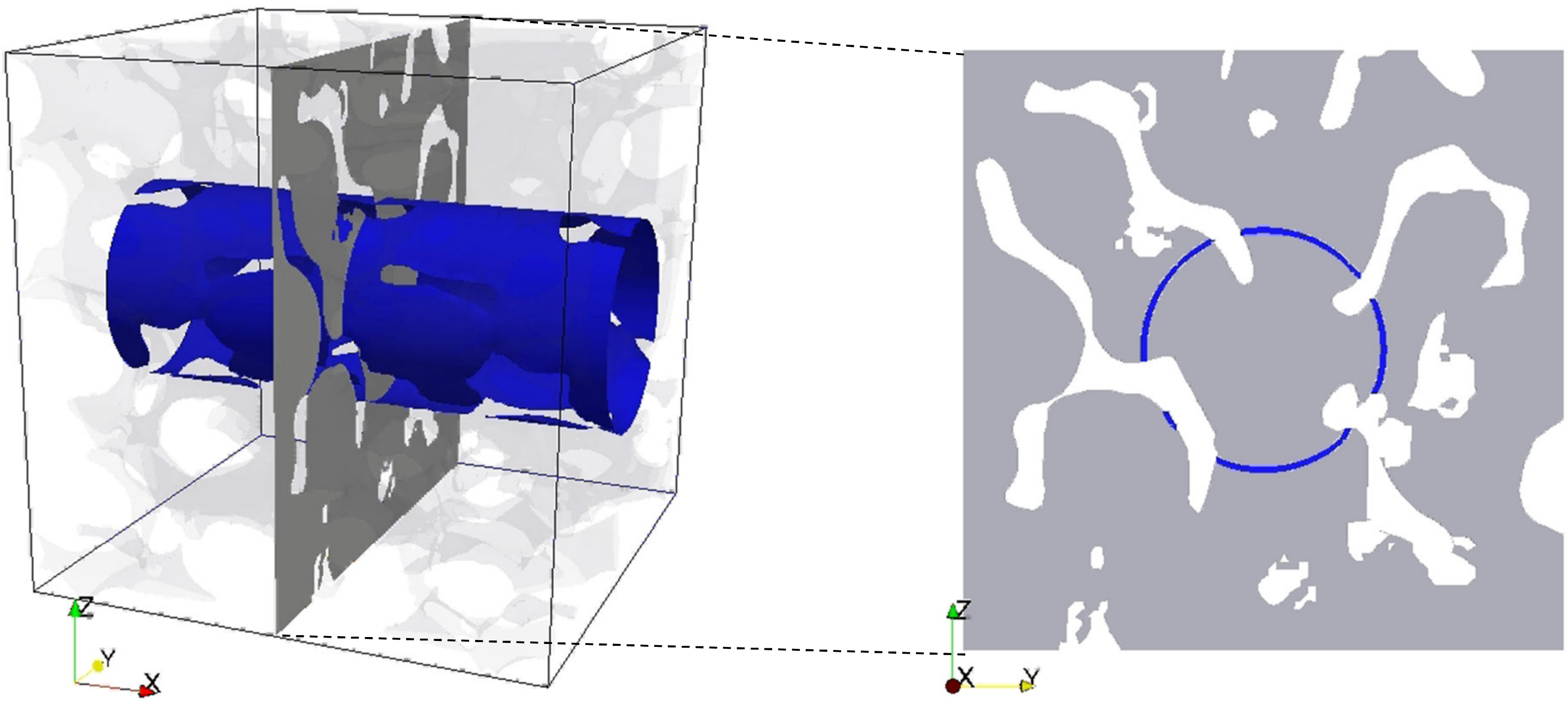
$$-\nabla p = -\nabla P + \mathbf{f}_x$$

- Input to DNS:
  - liquid saturation *ß* $(V_{liquid}) / (V_{liquid} + V_{gas})$
  - Pressure drop $\Delta p/\Delta x$



SiSiC foam, 20 ppi, 85% porosity
ß = 0.2
$\Delta p/\Delta x$ = 200 Pa/m

Interface-resolving for Two-phase Flow in Sponge

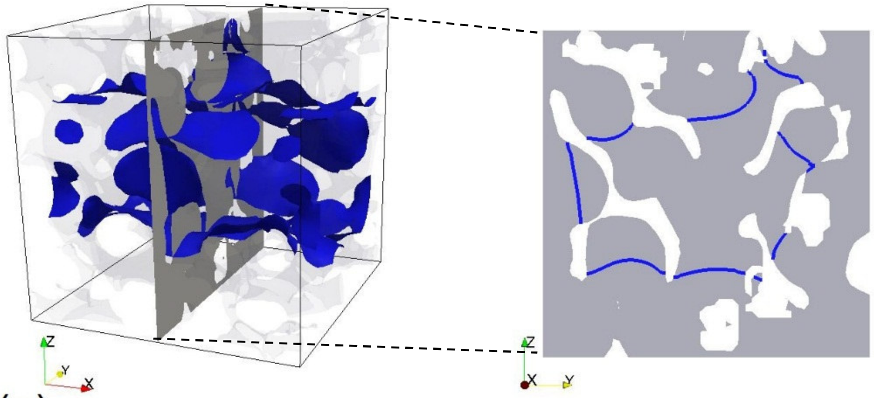


- Liquid saturation *ß* = 0.2 and $\Delta p/\Delta x$ = 200 Pa/m
- Equilibrium contact angle = 90°

Interface-resolving for Two-phase Flow in Sponge

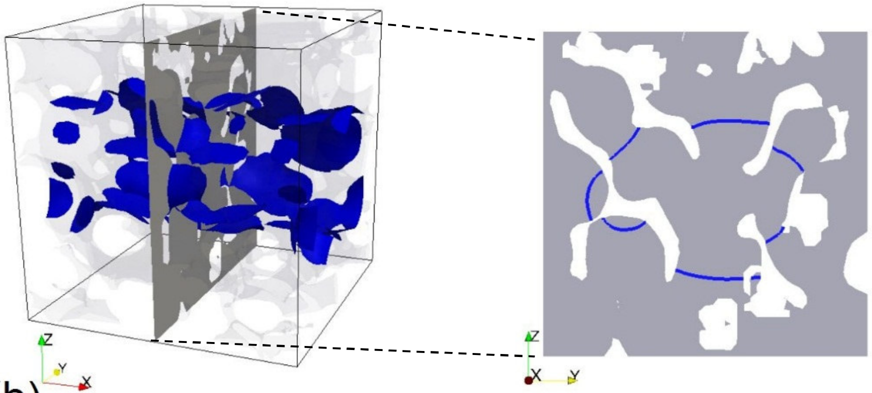
- Effect of equilibrium contact angle θ_e (i.e. solid surface wettability)

$\theta_e = 40°$



(a)

$\theta_e = 80°$

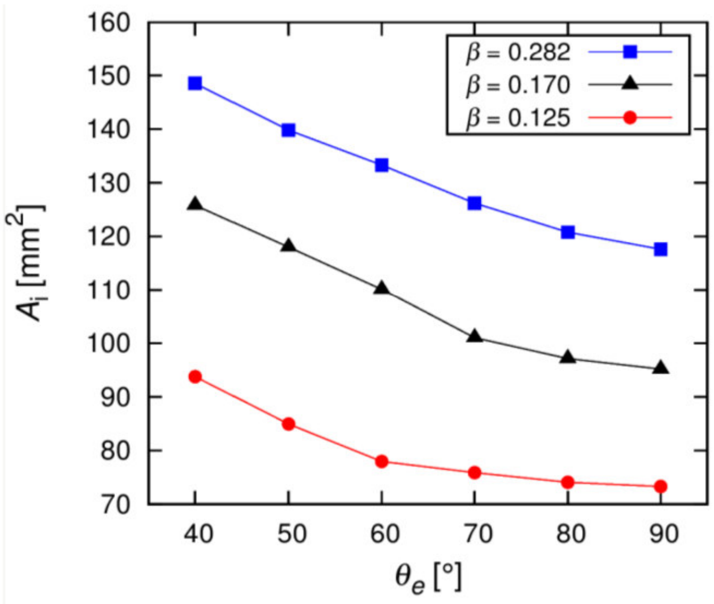


(b)

Interface-resolving for Two-phase Flow in Sponge

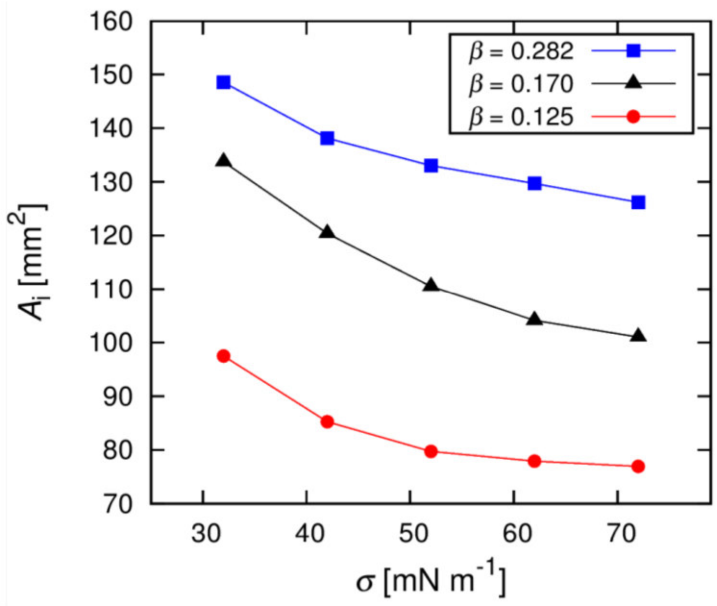
Karlsruhe Institute of Technology

Effect of contact angle



Gas-liquid interfacial area A_i vs. contact angle θ_e for different liquid saturation ß

Effect of gas-liquid surface tension



Gas-liquid interfacial area A_i vs. contact angle θ_e for different liquid saturation ß

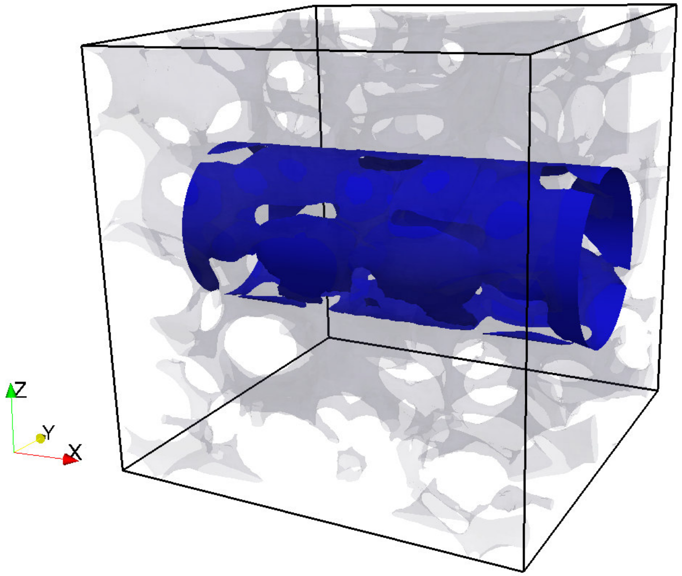
contact angle ↓
gas-liquid surface tension ↓

→ gas-liquid interfacial area ↑

→ Interfacial mass transfer ↑

Summary and Outlook

- Phase Field Method and *phaseFieldFoam* in OpenFOAM
  - Validation for droplet or bubble interacting with solid surface
- DNS for interface-resolving of gas-liquid flows in sponge structure
  - **Providing clear evidence that interfacial area can be increased by tuning surface wettability or interfacial tension**
- Outlook for future work:
  - Further investigations on other initialization strategy
  - Derive closure relation for Euler-Euler modeling and simulation
  - Experimental study on local interface distribution is highly needed



Acknowledgement

- PhD study funded by Germany Helmholtz Energy Alliance "Energy-efficient chemical multiphase processes"

- **Partners:**
  - Dr. H. Marschall
    (CSI, TU Darmstadt, Germany)
  - Dr. B. Dietrich, S. Meinicke
    (KIT-TVT, Karlsruhe, Germany)
  - Prof. B. Frohnapfel, V. Fink
    (KIT-ISTM, Karlsruhe, Germany)
  - Prof. P. Yue
    (Virginia Tech, USA)
  - Prof. H. Alla
    (USTO, Oran, Algeria)