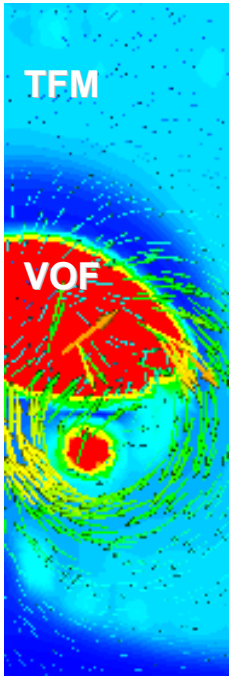
Numerical Simulation of Gas-Liquid-Reactors with Bubbly Flows using a Hybrid Multiphase-CFD Approach



Hybrid Interface Resolving Two-Fluid Model (HIRES-TFM) by Coupling of the Volume-of-Fluid (VOF) method and the Two-Fluid model (TFM)

using OpenFOAM

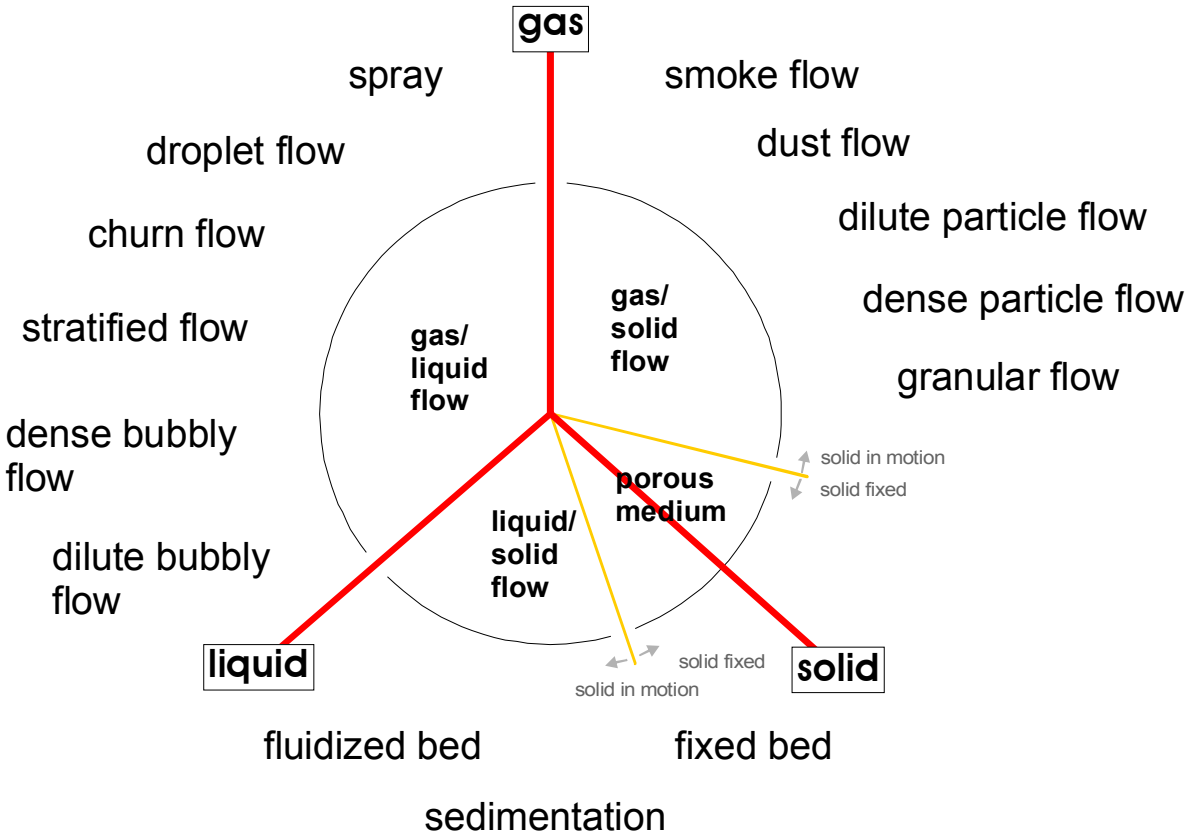
Dipl.-Ing. Holger Marschall
Chair of Chemical Engineering
Technische Universität München

Outline

- **background & motivation**
- **problem statement**
  - state-of-the-art (VOF & TFM)
  - hybrid approach (HIRES-TFM)
- **governing equations**
  - basic equation (VOF & TFM)
  - basic idea & switch criterion (HIRES-TFM)
- **numerical results**
  - prototype examples (HIRES-TFM)
- **outlook**

Background

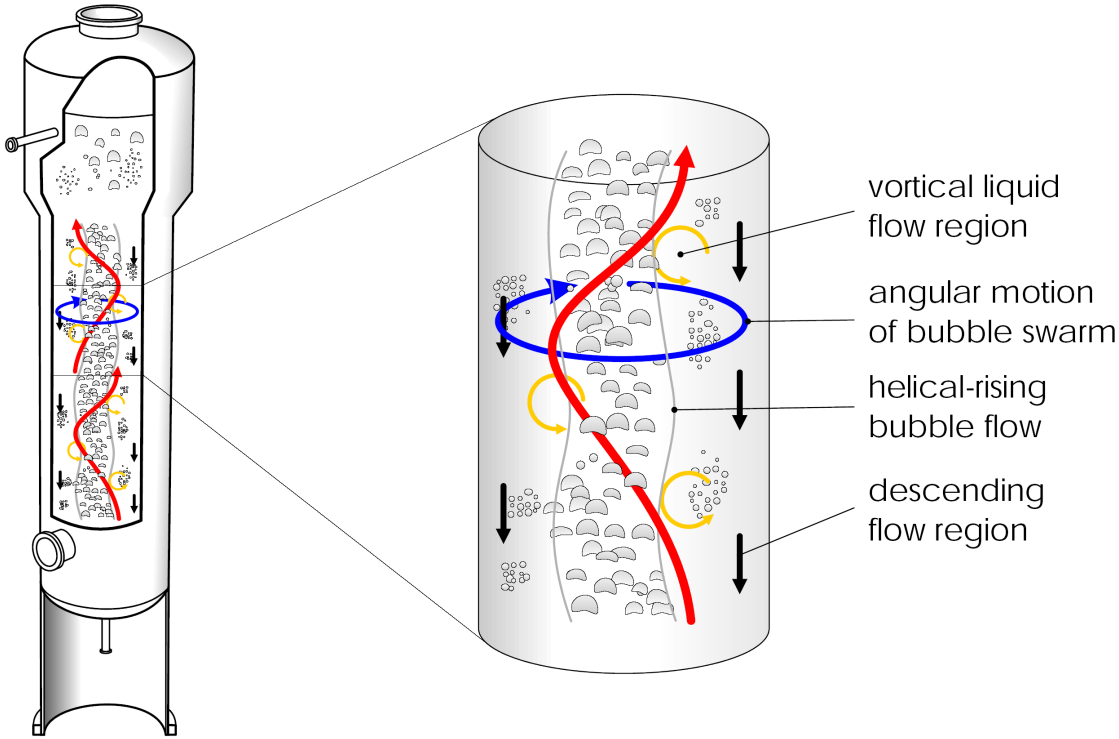
Phenomenology of Multiphase-Flows – Process Technology

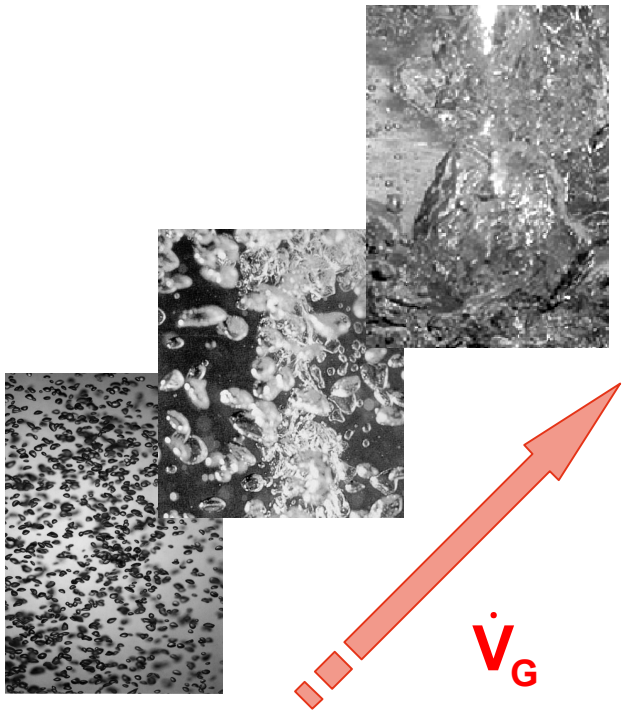


[Laurien, 2004]

Motivation

Phenomenology of Multiphase-Flows – Bubble Column Reactors

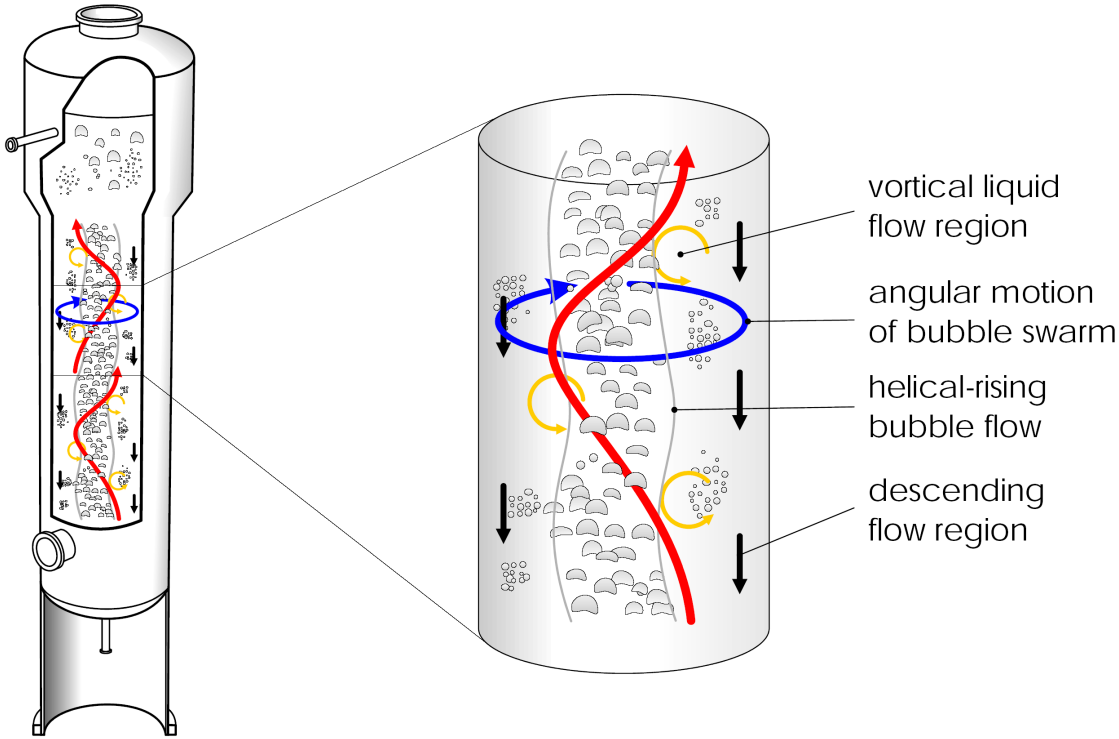




[Fan, 1990], [Mudde, 2003]

Motivation

Phenomenology of Multiphase-Flows – Bubble Column Reactors



- fluid dynamics of two-phase flow systems in process apparatus and chemical reactors with **transient flow structures**
- fluid dynamics, reaction and mass transfer at gas-liquid interfaces of two-phase flow systems with **spatial and/or temporal scales over more than 6 orders of magnitude**

[Fan, 1990], [Mudde, 2003]

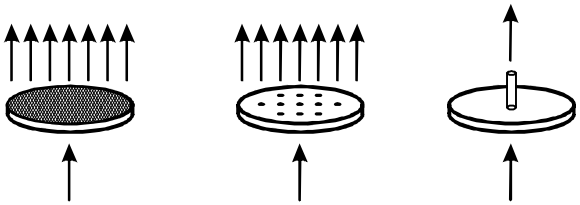
Problem Statement

State-of-the-Art – Current Frontiers

reactor inlet

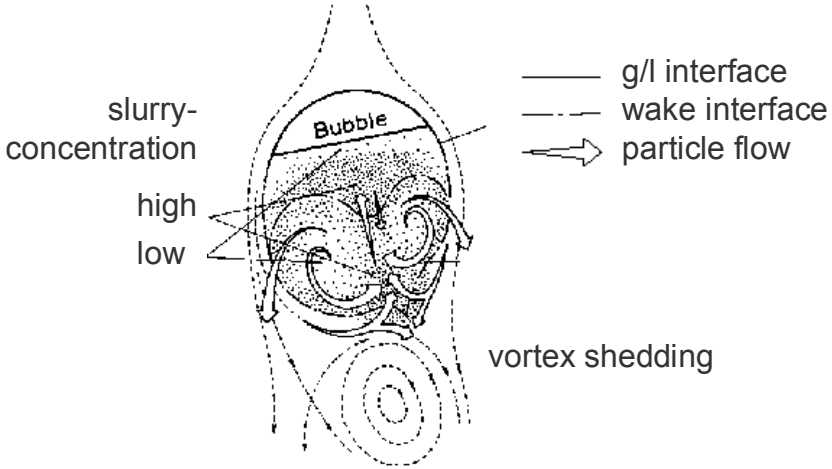
modelling, empiricism

- porous plates, perforated plates, single orifice nozzles
- multiple orifice nozzles, perforated rings, spider-type spargers



reactor interior

flow structure ↔ reactor performance



requirements

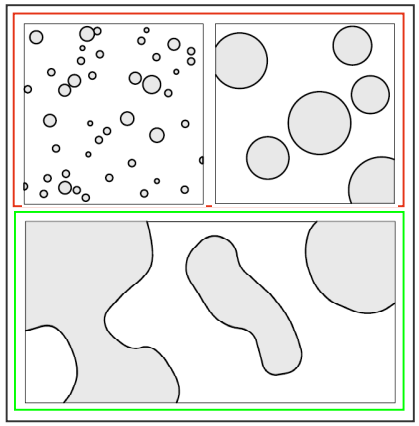
- Higher Accuracy, Cutback of Conservatisms & Uncertainties
- Portability to New Geometries and Range of Parameters
- Enhanced Scale-Up Options

[Deckwer, 1985], [Fan, 1990]

Problem Statement

State-of-the-Art – Hierarchy of Numerical Methods

macroscopic & mesoscopic level

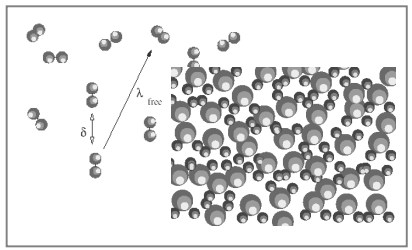


field averaging models (EE)

entity tracking models (EL)

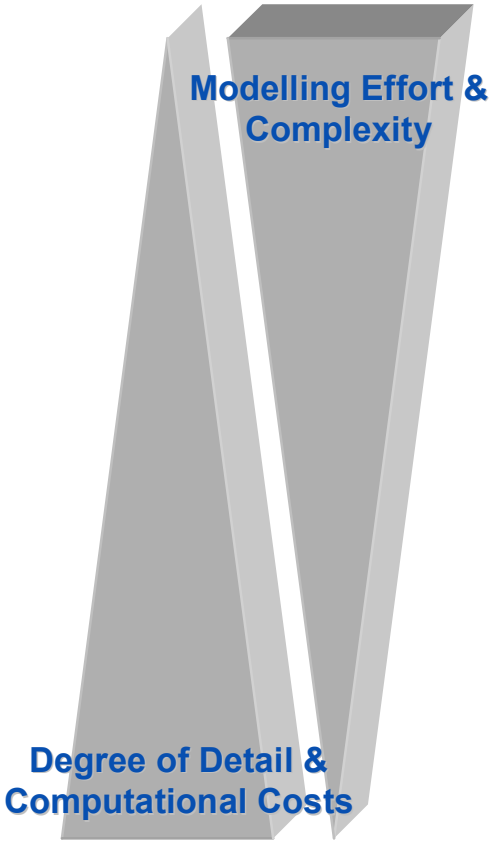
interface resolving methods (EE)

microscopic level



Lattice Boltzmann

Monte Carlo



[Paschedag, 2007]

Problem Statement
Hybrid Approach

→ **challenge**
- Multiscale CMFD
- Large-scale CMFD

→ **conceptual approach**
- adaptive:
  as coarse as possible &
  as detailed as required

Spatial Resolution	Method	Fundamental Eqs.	Applicability to Practical Problems
low ($\Delta x >> d$)*	Averaging Method (Homogeneous, Drift-Flux, Two-Fluid Models)	Averaged Field Eqs. + Constitutive Eqs.	high
intermediate ($\Delta x \sim d$)	Bubble Tracking Method (One-Way, Two-Way Methods)	Eq. of Bubble Motion + Constitutive Eqs.	intermediate
high ($\Delta x < d$)	Interface Tracking Method (Front Tracking, Volume Tracking, Level Set)	Navier-Stokes Eq. + Surface Tension	low
high ($\Delta x << d$)	Microscopic Method (Lattice Gas, Lattice Boltzmann Methods)	Translation & Collision of Pseudo Molecules	low

* d: bubble diameter, Δx: cell size

⇒ **HIRES-TFM = Hybrid Interface-Resolving Two-Fluid Model**
- **interface resolving algorithm VOF** for free surface flow regions
  as long as local computational grid density allows interface capturing
- **extended two-fluid model TFM** for dispersed flow regions
  where dimensions of fluid parts are comparable to or smaller than grid spacing

[Tomiyama, 1998]

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Hybrid Approach

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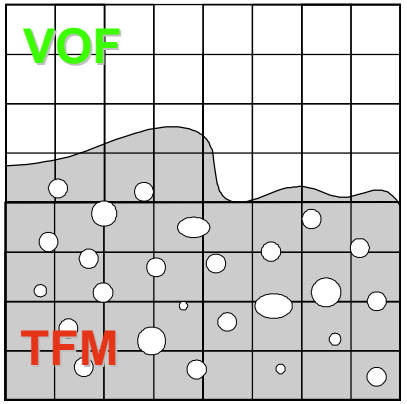

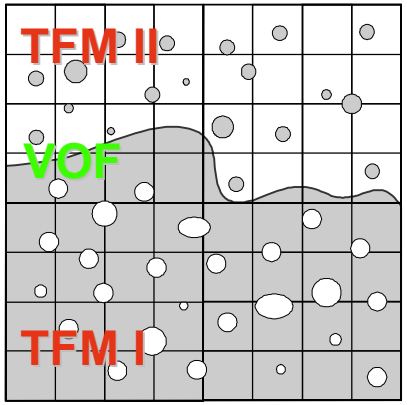

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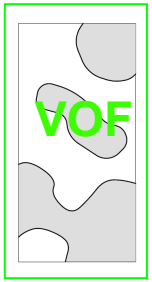
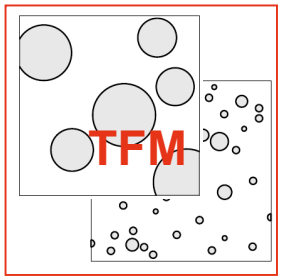
Problem Statement
Hybrid Approach

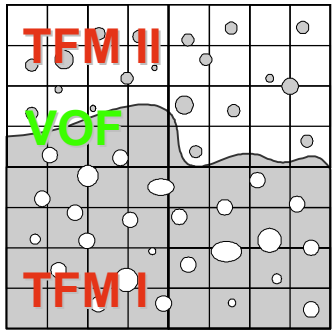
- interfacial friction
- interfacial tension
- turbulence
- mass transfer
- economic resolution of interfacial structures and dynamics: local adaptive mesh refinement (AMR)



interFoamExt



bubbleFoamExt



HIRES-TFM

- interfacial forces
  - drag force
  - non-drag forces
    (lift force, turbulent drag force)
- polydispersity
  - (class method)
  - (method of moments)
  - (Monte-Carlo method)
  - interfacial area conc.
- coalescence and breakup
- turbulence incl. BIT
- mass transfer

Governing Equation

Coupling of the VOF method and the TFM – basic equations

- continuity equation

$$\nabla \cdot \boldsymbol{U} = 0$$

- momentum equation

$$\frac{\partial \rho \boldsymbol{U}}{\partial t} + \nabla \cdot (\rho \boldsymbol{U}\boldsymbol{U}) = -\nabla p + \nabla \cdot \left[\mu \left(\nabla \boldsymbol{U} + \nabla \boldsymbol{U}^T \right) \right] + \rho \boldsymbol{g} + \boldsymbol{F}_\sigma$$

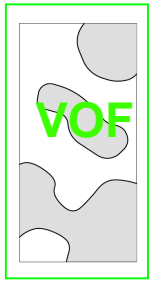
- topological equation (continuity)

$$\boxed{\frac{\partial \alpha}{\partial t} + \nabla \cdot (\boldsymbol{U}\alpha) = 0}$$

- mixture density & mixture viscosity

$$\mu = \alpha \mu_a + (1-\alpha)\mu_b$$

$$\rho = \alpha \rho_a + (1-\alpha)\rho_b$$

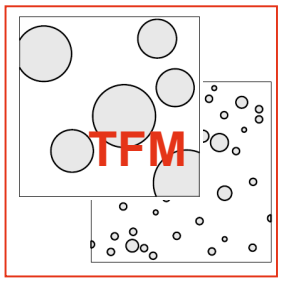


- phase fraction equation (continuity)

$$\boxed{\frac{\partial \alpha_\varphi}{\partial t} + \nabla \cdot \left(\bar{\boldsymbol{U}}_\varphi \alpha_\varphi \right) = 0}$$

- momentum equation

$$\frac{\partial \alpha_\varphi \bar{\boldsymbol{U}}_\varphi}{\partial t} + \nabla \cdot \left(\alpha_\varphi \bar{\boldsymbol{U}}_\varphi \bar{\boldsymbol{U}}_\varphi \right) + \nabla \cdot \left(\alpha_\varphi \bar{\boldsymbol{R}}_\varphi^{eff} \right) = -\frac{\alpha_\varphi}{\rho_\varphi} \nabla \bar{p} + \alpha_\varphi \boldsymbol{g} + \frac{\alpha_\varphi}{\rho_\varphi} \bar{\boldsymbol{M}}_\varphi$$



+ constitutive equations
  interfacial momentum transfer
+ model equation
  interfacial tension

Governing Equation

Coupling of the VOF method and the TFM – interface compression

- **problem of VOF methods:**
  accuracy and reliability of the numerical approach to ensure the interface remains sharp
- **basic idea for a sharp interface:**
  convective transport term, counter gradient (against num. diffusion), conservative & bounded

$$\nabla \cdot \left(\boldsymbol{U}_r \; \tilde{c}(1-\tilde{c}) \right)$$

- scalar flux second-moment closure in complex combustion models for turbulent flames

- $\boldsymbol{U}_r$ relative velocity between burnt and unburnt gases
- $\tilde{c}$ progress variable

Governing Equation

Coupling of the VOF method and the TFM – interface compression

- **problem of VOF methods:**
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- **basic idea for a sharp interface:**
  convective transport term, counter gradient (against num. diffusion), conservative & bounded

$$\frac{\partial \alpha_a}{\partial t} + \nabla \cdot \left(\bar{U}_a \alpha_a \right) + \nabla \cdot \left(\bar{U}_c \alpha_a \left(1 - \alpha_a \right) \right) = 0$$

$$\underbrace{\nabla \cdot \left(U_r \ \tilde{c}(1-\tilde{c}) \right)}$$

where $\bar{U}_c = c_\alpha \left| \bar{U} \right| \frac{\nabla \alpha_a}{\left| \nabla \alpha_a \right|}$

$$\bar{U}_c = \min\left[c_\alpha \left| \bar{U} \right|, \max\left(\bar{U} \right) \right] \frac{\nabla \alpha_a}{\left| \nabla \alpha_a \right|}$$

$$1 \le c_\alpha \le 4$$

- convection-based sharpening algorithm in the phase fraction equation for interface capturing

- $\bar{U}_c$ artificial compression term acting normal to the interface
- α_a volume fraction of phase a

Governing Equation

Coupling of the VOF method and the TFM – switch criterion

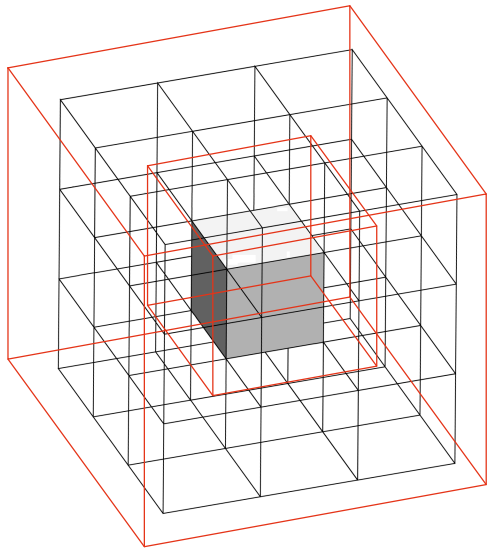
$$\frac{\partial \alpha_a}{\partial t} + \nabla \cdot \left(\bar{U}_a \alpha_a \right) + \bar{\Gamma}_d \; \nabla \cdot \left(\bar{U}_c \alpha_a \left(1 - \alpha_a \right) \right) = 0$$

Γ_d switch factor, that

$$\Gamma_d = f\left(\alpha_a, \nabla \alpha_a, a_i, \Delta V, \ldots, We \right)$$

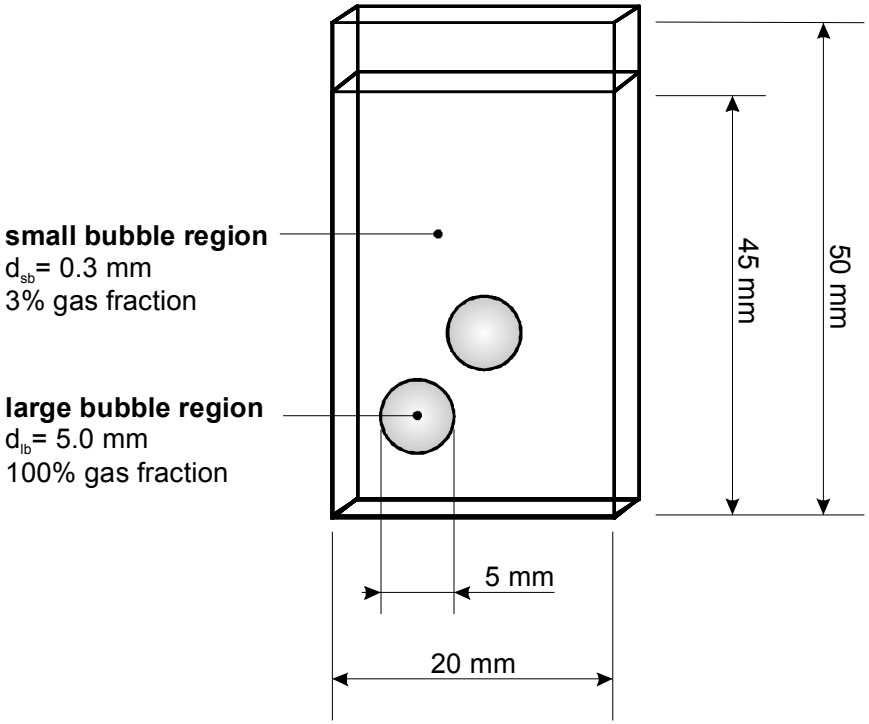
- … carries the information about the interface shape
- …quantifies the local dispersion of the two-phase flow structure
- …estimates the interface reconstruction correctness of the VOF method

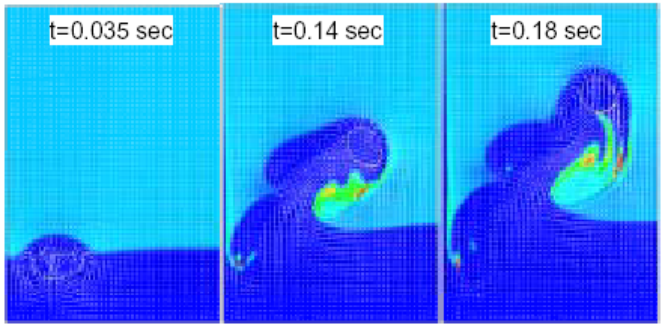
$$\bar{\Gamma}_d = \frac{\sum_{nb} \Gamma_d A_i}{\sum_{nb} A_i}$$



Numerical Results

- **Prototype Examples – HIRES-TFM**

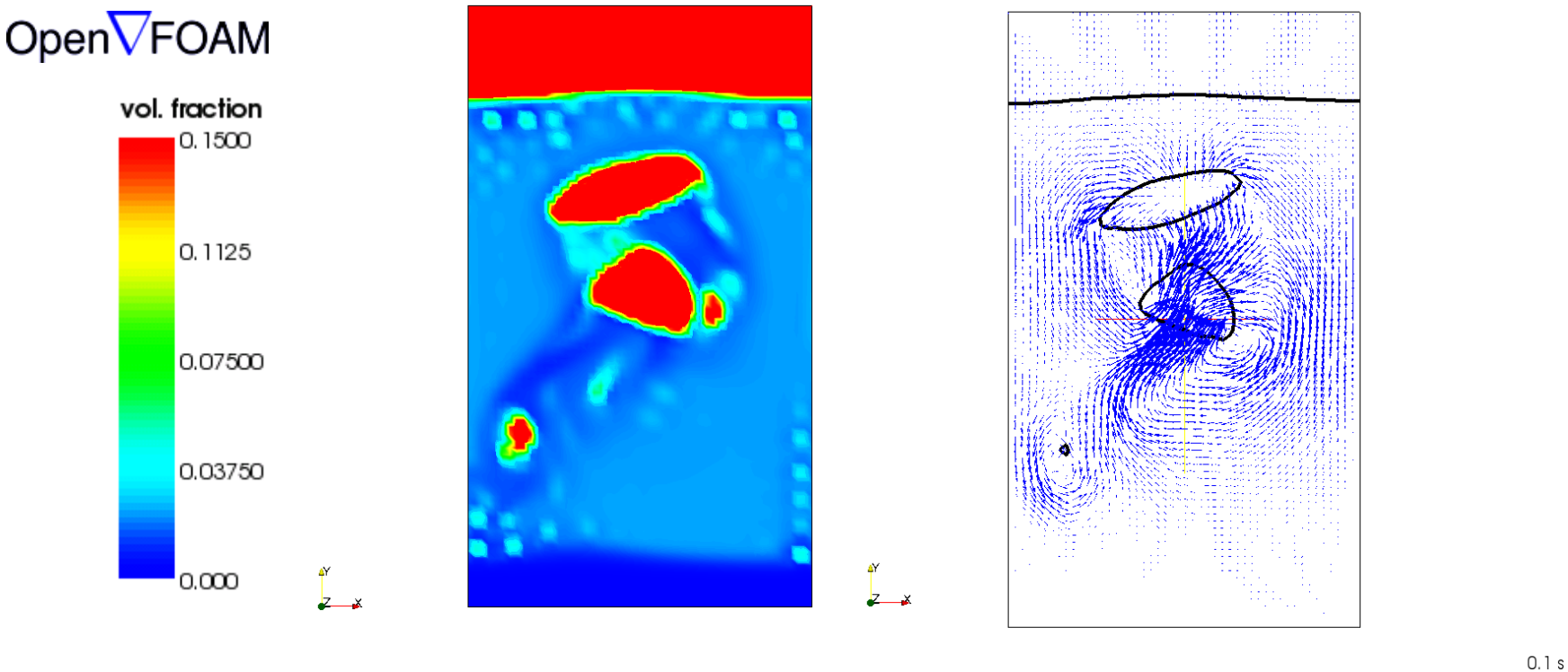




Interaction among a 5 mm bubble and many small bubbles of 0.25 mm in diameter in a 2D air-water system **[Tomiyama, 2003]**

Numerical Results

- **Prototype Examples – HIRES-TFM**



Numerical Results

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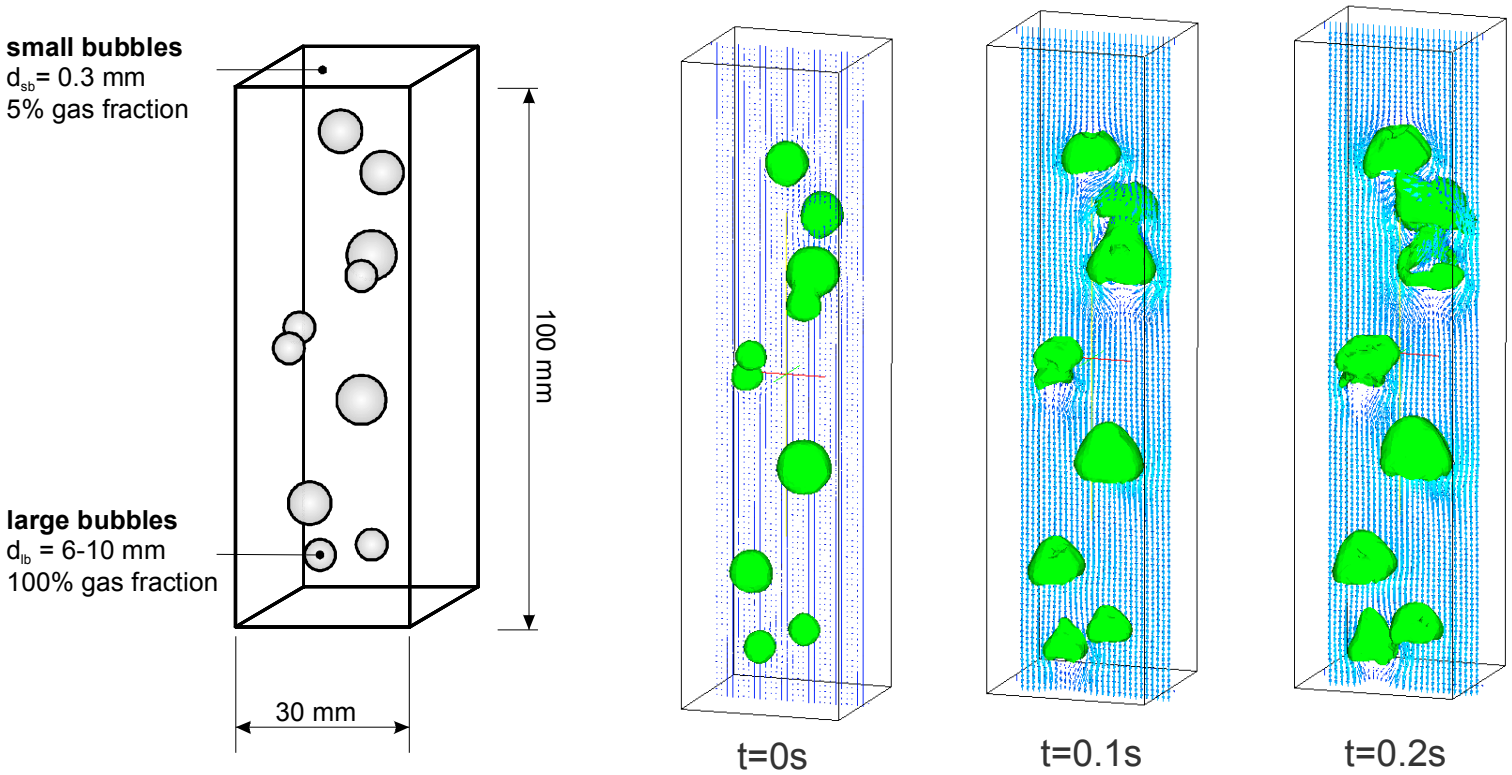
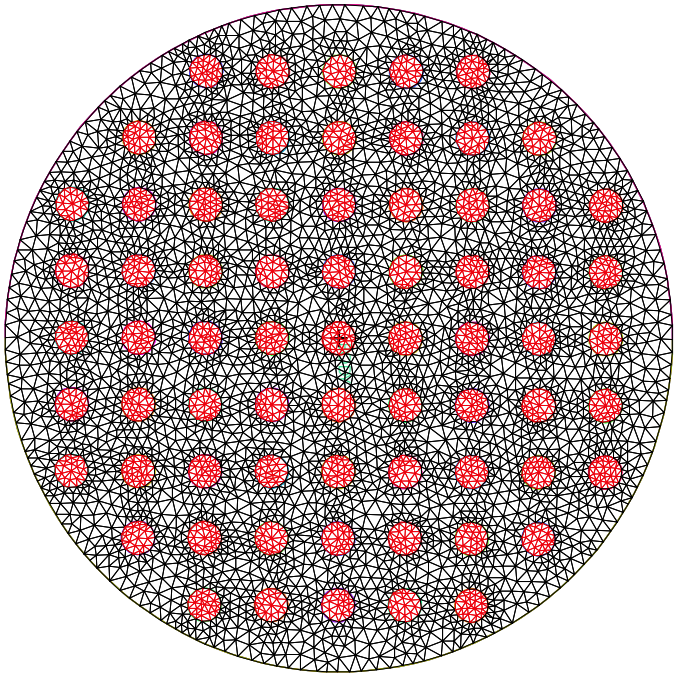


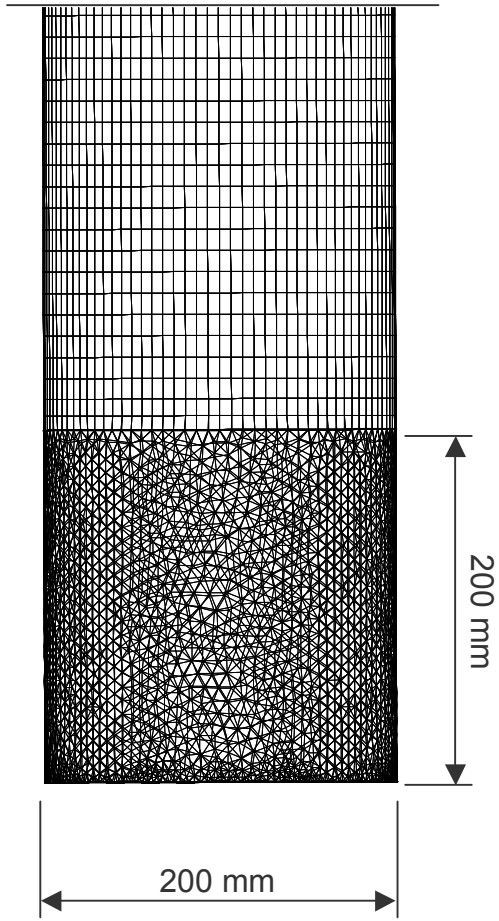
Outlook

- **Plans – HIRES-TFM**

simulation of a lab-scale bubble column with sparger

vs. experimental validation

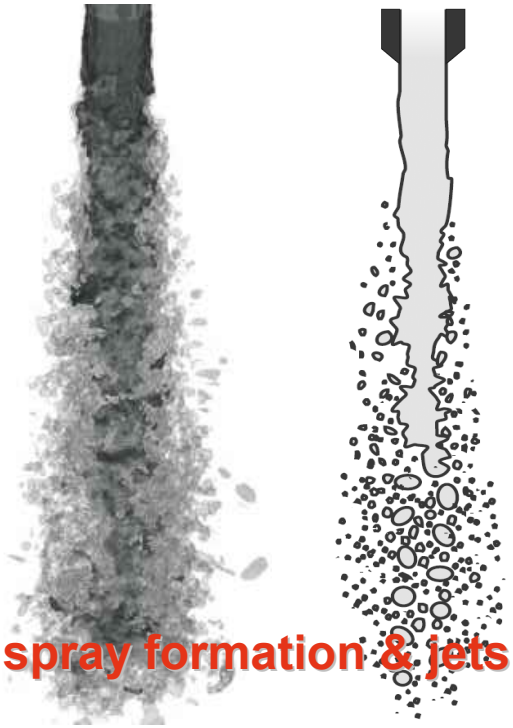


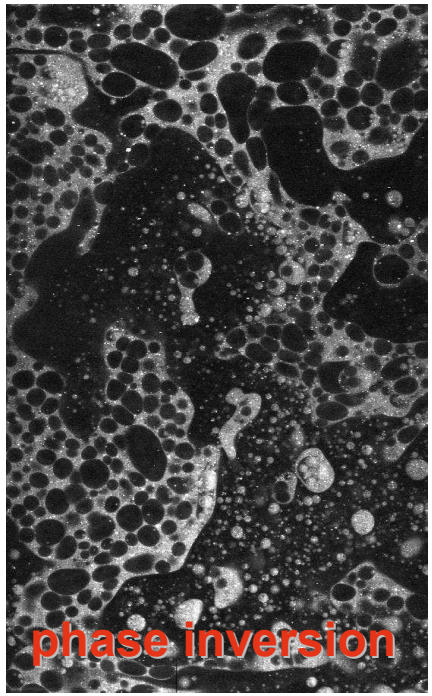


H = 2000 mm
D = 200 mm
d_h = 10 mm

Outlook

- **Future Challenges – HIRES-TFM**





Thanks for your attention…

- **Acknowledgements**

  – Prof. Dr.-Ing. Olaf Hinrichsen & Prof. Wolfgang Polifke (TU München)
  – Dr. Henry G. Weller (OpenCFD Ltd.)
  – Prof. Dr. Hrvoje Jasak (FSB Zagreb, Wikki Ltd.)

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