Critical assessment of statistical turbulence models for bubble-driven flows

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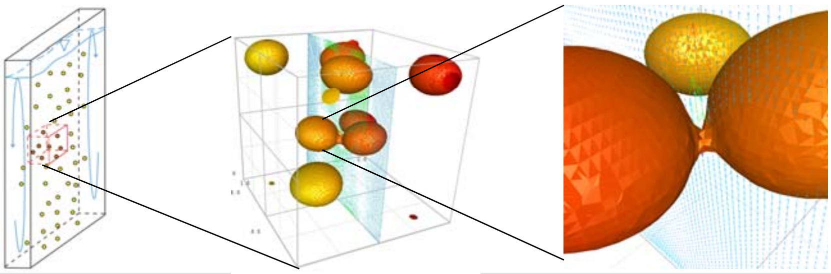

KIT – University of the State of Baden-Wuerttemberg and
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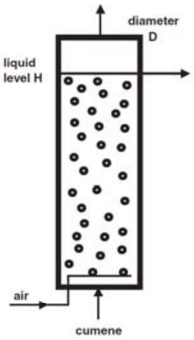
Outline

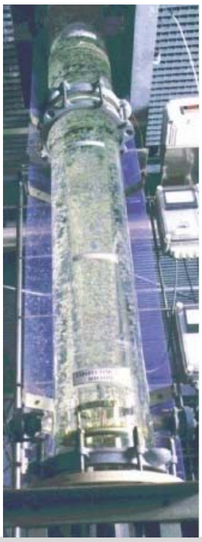
- Introduction
- CFD methods for bubble columns
- Model limitations
    - Turbulence in bubbly flows
    - Interaction between closure relations
- Development of improved models by DNS
    - Previous results for k_L equation
    - Ongoing work within BMBF project Multiphase
- Outlook

Introduction

- Applications/devices with bubble-driven gas-liquid flows
  - Waste water treatment
  - Nuclear power plants
  - Chemical reactors
    - Ail lift reactors
    - Bubble column reactors
- <u>Bubble column reactors</u>
  - Volume 0.01 – 3000 m^3
  - Diameter 0.2 – 20 m
  - Height to diameter ratio 3 – 10
  - High pressure, high temperature
  - Reactions of organic liquids
    - Oxidations, hydrogenations, …
    - Example: oxidation of cumene for production of phenol (a precursor to plastics)

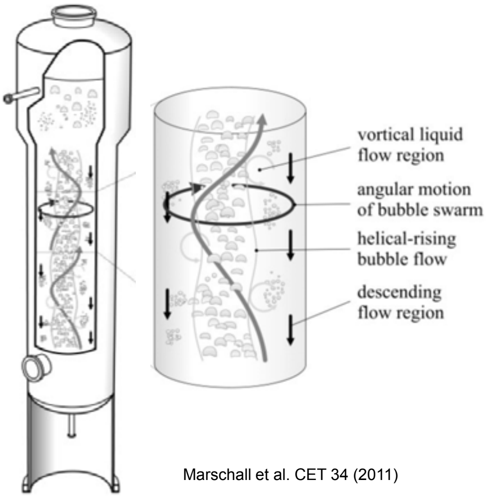


M. Weber, CET 25 (2002)



Flow features in bubble columns

- Rising bubbles drive recirculating liquid flow (upward in center, downward near wall) and generate bubble-induced turbulence (also called pseudo-turbulence)
- Recirculating liquid flow generates shear-induced turbulence which interacts with the pseudo-turbulence
- Turbulence influences collision and breakup of bubbles which results in a spectrum of bubble sizes (heterogeneous regime)



Marschall et al. CET 34 (2011)

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CFD methods for bubble columns

- Length scales
  - Column diameter d_C = 0.2 – 20 m
  - Bubble diameter d_B = 1 – 10 mm

  → d_C / d_B = 200 – 2000

  → *Direct numerical simulation is impossible (and also not meaningful)*
- Time scales
  - Liquid recirculation time and bubble residence time are much larger than the time scale of bubble motion d_b/U_B

  → *Large-eddy-simulations is impossible (a huge problem time is required to achieve reliable statistics)*
- Gas holdup up to 40% → *Euler-Lagrange approach is not meaningful*
- Typical simulation turn around time requested by industry 1 - 3 days
- Euler-Euler approach based on Reynolds-averaged Navier-Stokes equations is the only approach that can meet industrial demands
  - Reynolds stress models
  - Two-equation eddy viscosity models (k-ε, k-ω, SST, …)
- *CFD is not yet used as tool for design of industrial scale bubble columns*

Common model approaches

- Modeled k_L equation is solved (with or without two-phase specific interfacial term) while turbulence in gas phase is neglected
- Both, the modeled k_L and k_G equations are solved (with or without two-phase specific interfacial term)
- The modeled k_L equation is solved without interfacial term and the bubble-induced turbulence is taken into account by an extra contribution to the eddy viscosity (e.g. by the model of Sato)
- It is common practice to adopt single phase closure laws with single phase coefficient sets (e.g. standard, RNG, realizable *k*-*ε*, low *Re*, …)
  - Motivation: in limit $\alpha_G \to 0$ the model must reduce to single phase version
  - However, model coefficients are not universal even for single phase flow
- Status of model development
  - Computations with model variants are compared with experimental data (mean flow is often well described, but not turbulence quantities)
  - Useful to identify which models performs best for a certain experiment but hardly useful for development of physically sound improved closure relations

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Turbulence in bubbly flows

- Pool of stagnant liquid
  - Rising bubbled induce pseudo-turbulence (displacement of liquid, bubble wakes)
  - Non-Gaussian probability density function
  - Spectrum follows a power law with slope -3 (this is attributed to bubble wakes)
- Turbulent pipe flow
  - Wall or core peaking ⇒ modulation of mean liquid velocity by bubbles
  - Bubbles can enhance or attenuate liquid turbulence as compared to single phase flow with same liquid flow rate
  - Spectrum exhibits different ranges (-5/3, -3)

- Neither pure pseudo-turbulence (bubble-induced turbulence) is fully understood nor how it modifies shear turbulence
- In bubble columns, there is an inherent non-linear interaction between bubble-induced and shear-induced turbulence

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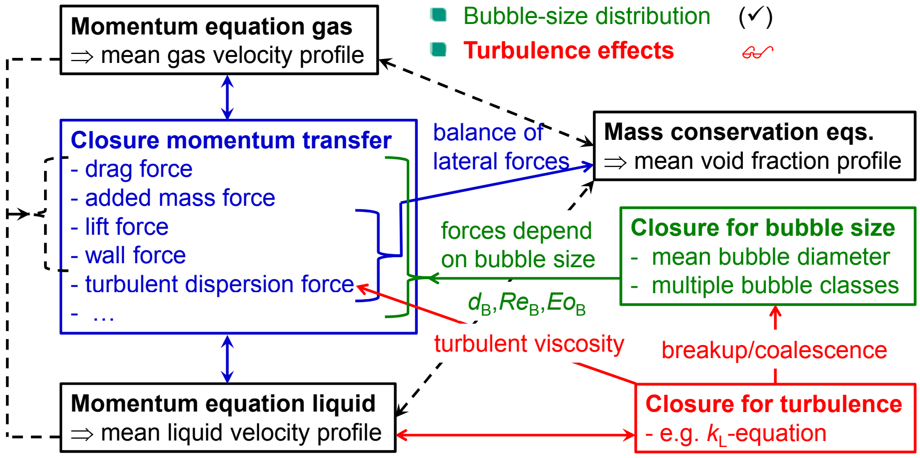
Interaction of closure relations

- **Closure relations in two-fluid model**
  - Interfacial transfer terms ✓
  - Bubble-size distribution (✓)
  - **Turbulence effects** 👓



Momentum equation gas
⇒ mean gas velocity profile

Closure momentum transfer
- drag force
- added mass force
- lift force
- wall force
- turbulent dispersion force
- …

balance of lateral forces

Mass conservation eqs.
⇒ mean void fraction profile

forces depend on bubble size

Closure for bubble size
- mean bubble diameter
- multiple bubble classes

d_B, Re_B, Eo_B

turbulent viscosity

breakup/coalescence

Momentum equation liquid
⇒ mean liquid velocity profile

Closure for turbulence
- e.g. k_L-equation

Exact analytical k_L equation

$$k_\mathrm{L} = \frac{1}{2}\overline{\overline{\mathbf{u}'_\mathrm{L} \cdot \mathbf{u}'_\mathrm{L}}}$$

$$\boxed{\begin{aligned} \frac{\partial}{\partial t}(\alpha_\mathrm{L} k_\mathrm{L}) + \nabla \cdot \left(\alpha_\mathrm{L} k_\mathrm{L} \overline{\overline{\mathbf{u}_\mathrm{L}}}\right) = {} & \underbrace{\frac{1}{Re_\mathrm{ref}} \nabla \cdot \left(\alpha_\mathrm{L} \overline{\overline{\tau'_\mathrm{L} \cdot \mathbf{u}'_\mathrm{L}}}\right) - \nabla \cdot \left[\alpha_\mathrm{L}\left(\overline{\overline{p'_\mathrm{L}\mathbf{u}'_\mathrm{L}}} + \frac{1}{2}\overline{\overline{\mathbf{u}'^2_\mathrm{L}\mathbf{u}'_\mathrm{L}}}\right)\right]}_{DIFFUSION} \\ & \underbrace{-\alpha_\mathrm{L}\overline{\overline{\mathbf{u}'_\mathrm{L}\mathbf{u}'_\mathrm{L}}} : \nabla\overline{\overline{\mathbf{u}_\mathrm{L}}}}_{PRODUCTION\ BY\ SHEAR} \underbrace{- \frac{1}{Re_\mathrm{ref}}\alpha_\mathrm{L}\overline{\overline{\tau'_\mathrm{L} : \nabla\mathbf{u}'_\mathrm{L}}}}_{DISSIPATION} + \underbrace{\overline{\left[\frac{1}{Re_\mathrm{ref}}\tau'_\mathrm{L,i} - p'_\mathrm{L,i}\mathbb{I}\right] \cdot \mathbf{u}'_\mathrm{L,i} \cdot \hat{\mathbf{n}}_\mathrm{L,i} a_\mathrm{i}}}_{PRODUCTION\ BY\ INTERFACIAL\ TERM} \end{aligned}}$$

Kataoka & Serizawa (1989)

- All terms on the right hand side must be modeled
- All terms involve correlations between various fluctuating quantities or their gradients which can hardly be measured in non-dilute bubbly flow
- Here: use DNS to obtain insight in budget of k_L and perform a-priori tests of performance of models for individual closure terms

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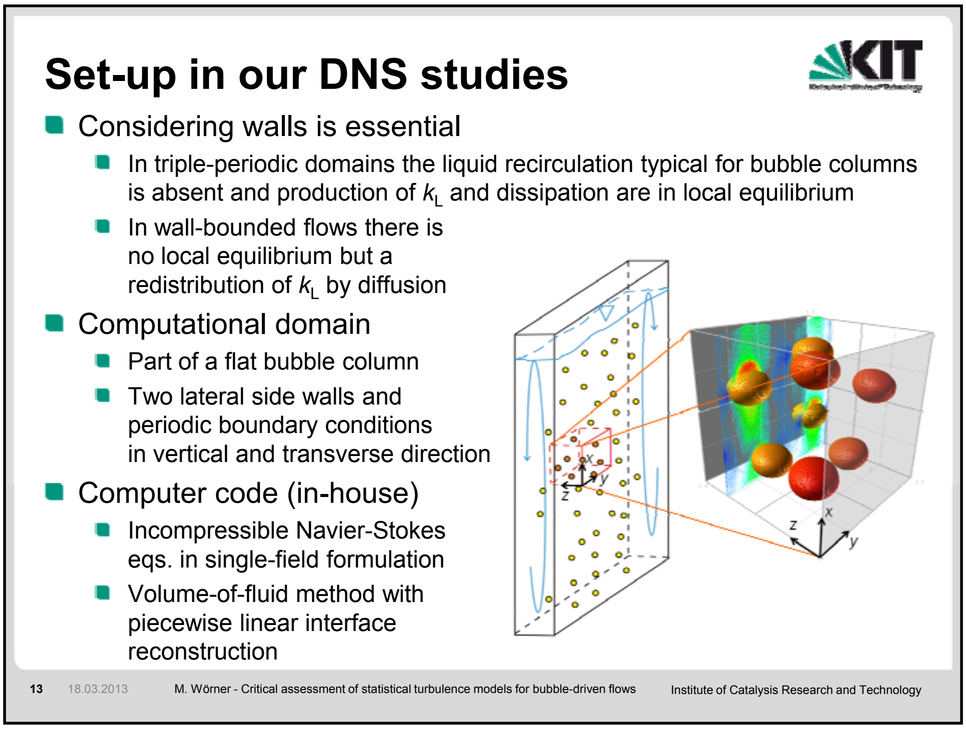
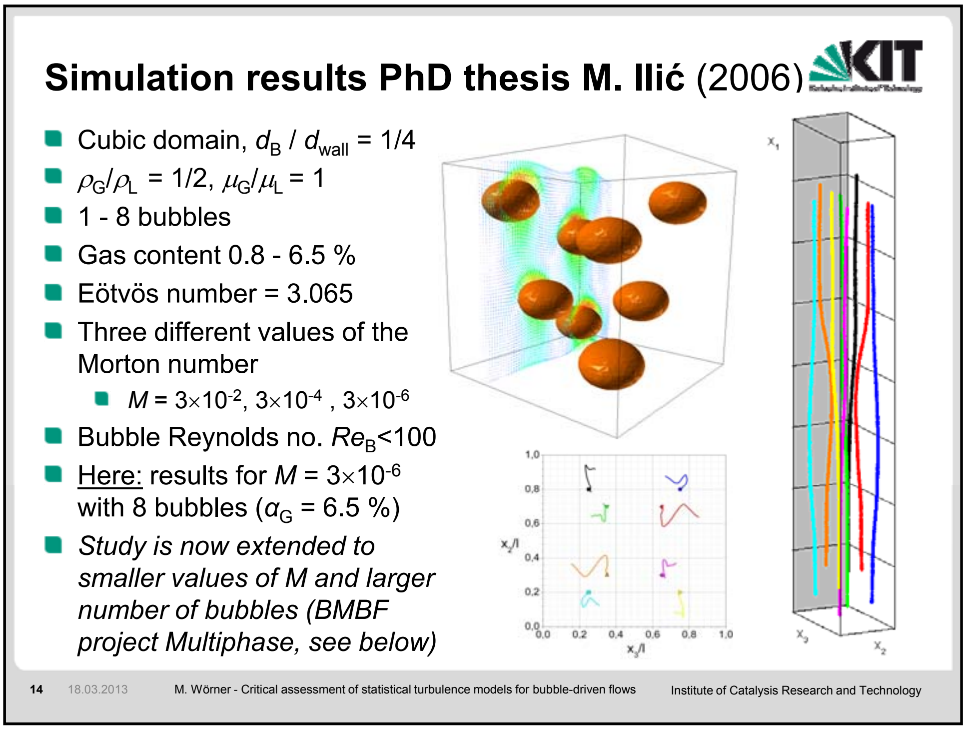


Set-up in our DNS studies

- Considering walls is essential
  - In triple-periodic domains the liquid recirculation typical for bubble columns is absent and production of k_L and dissipation are in local equilibrium
  - In wall-bounded flows there is no local equilibrium but a redistribution of k_L by diffusion
- Computational domain
  - Part of a flat bubble column
  - Two lateral side walls and periodic boundary conditions in vertical and transverse direction
- Computer code (in-house)
  - Incompressible Navier-Stokes eqs. in single-field formulation
  - Volume-of-fluid method with piecewise linear interface reconstruction

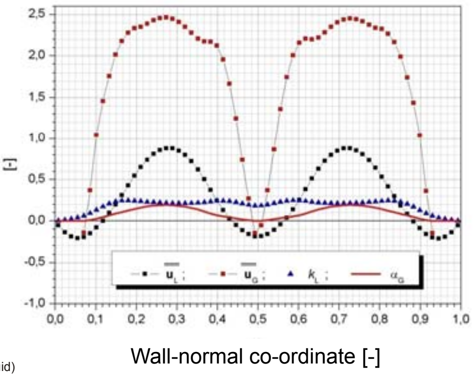


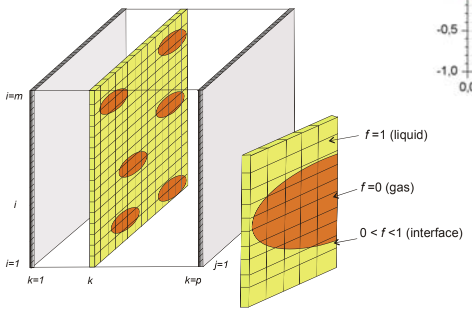
Simulation results PhD thesis M. Ilić (2006)

- Cubic domain, d_B / d_{wall} = 1/4
- ρ_G/ρ_L = 1/2, μ_G/μ_L = 1
- 1 - 8 bubbles
- Gas content 0.8 - 6.5 %
- Eötvös number = 3.065
- Three different values of the Morton number
  - $M = 3\times10^{-2}, 3\times10^{-4}, 3\times10^{-6}$
- Bubble Reynolds no. Re_B<100
- Here: results for $M = 3\times10^{-6}$ with 8 bubbles (α_G = 6.5 %)
- *Study is now extended to smaller values of M and larger number of bubbles (BMBF project Multiphase, see below)*

Averaging of simulation results

- Averaging over planes parallel to the side walls (statistically homogeneous)
- Additional averaging over different instants in time
- ⇒ wall normal profiles





Phase-average

$$\overline{\overline{A}}_{\mathrm{L};k} = \frac{\sum_{i,j} f_{i,j,k} A_{\mathrm{L};i,j,k}}{\sum_{i,j} f_{i,j,k}}$$

Phase-fluctuation

$$A'_{\mathrm{L};i,j,k} = A_{\mathrm{L};i,j,k} - \overline{\overline{A}}_{\mathrm{L};k}$$

Budget of exact k_L-equation

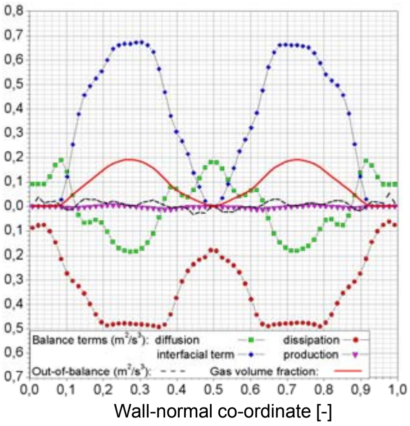
$$\frac{\partial}{\partial t}\left(\alpha_{\mathrm{L}} k_{\mathrm{L}}\right) + \nabla\cdot\left(\alpha_{\mathrm{L}} k_{\mathrm{L}} \overline{\overline{\mathbf{u}_{\mathrm{L}}}}\right) =$$

$$\underbrace{\frac{1}{Re_{\mathrm{ref}}}\nabla\cdot\left(\alpha_{\mathrm{L}}\overline{\overline{\mathbb{T}'_{\mathrm{L}}\cdot\mathbf{u}'_{\mathrm{L}}}}\right) - \nabla\cdot\left[\alpha_{\mathrm{L}}\left(\overline{\overline{p'_{\mathrm{L}}\mathbf{u}'_{\mathrm{L}}}} + \frac{1}{2}\overline{\overline{(\mathbf{u}'_{\mathrm{L}}\cdot\mathbf{u}'_{\mathrm{L}})\mathbf{u}'_{\mathrm{L}}}}\right)\right]}_{DIFFUSION}$$

$$\underbrace{-\alpha_{\mathrm{L}}\overline{\overline{\mathbf{u}'_{\mathrm{L}}\mathbf{u}'_{\mathrm{L}}}} : \nabla\overline{\overline{\mathbf{u}_{\mathrm{L}}}}}_{PRODUCTION}$$

$$\underbrace{-\frac{1}{Re_{\mathrm{ref}}}\alpha_{\mathrm{L}}\overline{\overline{\mathbb{T}'_{\mathrm{L}} : \nabla\mathbf{u}'_{\mathrm{L}}}}}_{DISSIPATION}$$

$$\underbrace{+\overline{\left[\frac{1}{Re_{\mathrm{ref}}}\mathbb{T}'_{\mathrm{L;in}} - p'_{\mathrm{L;in}}\mathbb{I}\right]\cdot\mathbf{u}'_{\mathrm{L;in}}\cdot\mathbf{n}_{\mathrm{L;in}}a_{\mathrm{in}}}}_{INTERFACIAL\ \ TERM}$$



- Interfacial term is main source (production by shear is negligible here)
- No local equilibrium between production and dissipation
- Redistribution from core to wall by diffusion (pressure term > triple correl.)

A priori test of closure assumptions

- For each closure term, the profile predicted by different models is compared with the exact profile of the closure term as evaluated from the DNS data
- Main findings of the evaluation of model assumptions by Ilić
  - Interfacial term: modeling as work of drag force together with Tomiyama correlation for C_D shows good performance for all Morton numbers

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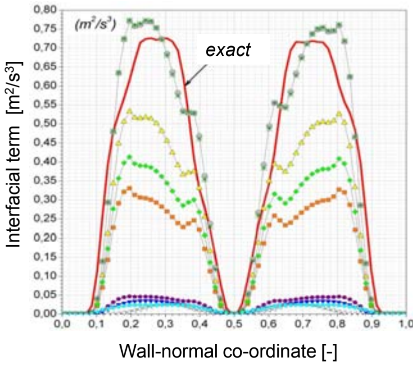
Models for interfacial term

exact: $-\overline{p'_{L,in} u'_{Li,in} n_{Li} a_{in}} + \overline{\tau'_{Lij,in} u'_{Li,in} n_{Lj} a_{in}}$

CLOSURE ASSUMPTIONS		
DRAG CONTRIBUTION Defined in the form of:	*Other contributions*	*Model of:*
Mean quantities:		
As power of drag force		
$W_D = 0.75 C_D \alpha_G \rho_L \lvert\overline{\overline{\mathbf{u}}}_r\rvert^3 / d_B$	$M_{vm}\overline{\overline{\mathbf{u}}}_r$ *none*	*Morel* ● *Troshko&Hassan* ✳
As part of power of drag force		
$0.05\alpha_G W_D$	*none*	*Boisson et al.* ⬟
$0.75 W_D$	*none*	*Olmos et al.* ▲
$1.44 W_D$	*none*	*Pfleger et al.* ■
$0.075 W_D$	$\alpha_G \rho_L k_L^{2/3} / d_B$	*Kataoka et al.* ◁
Drag force not explicitly included:		
$0.25\alpha_L \alpha_G \rho_L \left(1 + C_D^{4/3}\right) \lvert\overline{\overline{\mathbf{u}}}_r\rvert^3 / d_B$	*none*	*Lahey et al.* ◆
Mean and turbulent quantities:		
Only liquid turbulence properties $0.45 C_D \alpha_G \rho_L k_L \lvert\overline{\overline{\mathbf{u}}}_r\rvert / d_B$	$2.53\alpha_G \alpha_L \Pi$	*Sheng et al.* ▼
Turbulence properties of both phases $\frac{3}{4} C_D \frac{\lvert\overline{\overline{\mathbf{u}}}_r\rvert}{d_B} \left\{ 2\alpha_G \rho_L (C_t - 1) k_L - \frac{\nu_L^{k\varepsilon} \overline{\overline{\mathbf{u}}}_r \nabla \alpha_G}{\alpha_L \alpha_G} \right\}$	*none*	*Hill et al.* ●

C_D = drag coefficient (different formulations used)

$$C_t = \overline{u'_G u'_G} / \overline{u'_L u'_L} \propto f(l_e, Re_t, \alpha_G, d_B, \overline{\overline{\mathbf{u}}}_r, C_D)$$



Modeling of interfacial term as power of drag force gives good results in combination with C_D model of Tomiyama

$$C_D = \max\left\{ \min\left[\frac{16}{Re_B}\left(1 + 0.15 Re_B^{0.687}\right), \frac{48}{Re_B} \right], \frac{8}{3} \frac{Eö_B}{Eö_B + 4} \right\}$$

A priori test of closure assumptions

- For each closure term, the profile predicted by different models is compared with the exact profile of the closure term as evaluated from the DNS data
- Main findings of the evaluation of model assumptions by Ilić
  - Interfacial term: modeling as work of drag force together with Tomiyama correlation for C_D shows good performance for all Morton numbers
  - Production term and diffusion term: poor performance of standard single-phase type models (shear production term is strongly overestimated, diffusion term is strongly underestimated)
- The impact of any potential model improvement derived from DNS data is hard to assess in engineering CFD computations where the results are influenced by the non-linear interaction between models for bubble forces, bubble size distribution and turbulence. Development of improved models for BIT is an iterative process and requires detailed experimental data for various scale bubble columns for validation.
  $\Rightarrow$ **BMBF project Multi-Phase**

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BMBF project Multiphase

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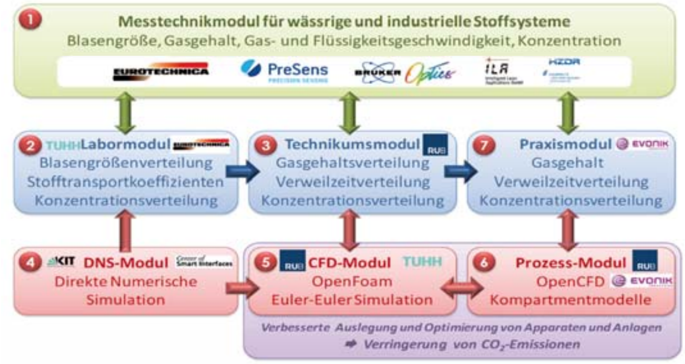
- **Multiscale modeling of multiphase reactors**
  (coordinated by Dr. M. Becker, Evonik industries)



① Messtechnikmodul für wässrige und industrielle Stoffsysteme
Blasengröße, Gasgehalt, Gas- und Flüssigkeitsgeschwindigkeit, Konzentration

② TUHH Labormodul
Blasengrößenverteilung
Stofftransportkoeffizienten
Konzentrationsverteilung

③ Technikumsmodul
Gasgehaltsverteilung
Verweilzeitverteilung
Konzentrationsverteilung

⑦ Praxismodul
Gasgehalt
Verweilzeitverteilung
Konzentrationsverteilung

④ KIT DNS-Modul
Direkte Numerische
Simulation

⑤ CFD-Modul TUHH
OpenFoam
Euler-Euler Simulation

⑥ Prozess-Modul
OpenCFD
Kompartmentmodelle

Verbesserte Auslegung und Optimierung von Apparaten und Anlagen
➡ Verringerung von CO_2-Emissionen

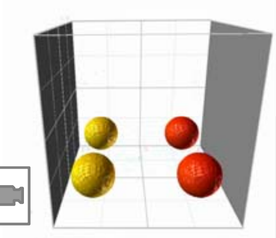
- One of the main goals of the project: Development of reliable multi-scale models which allow the numerical investigation and optimization of industrial scale multiphase reactors

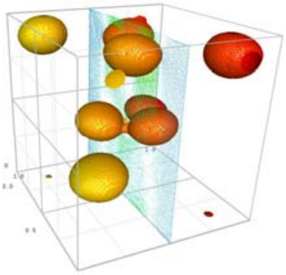
BMBF project Multiphase

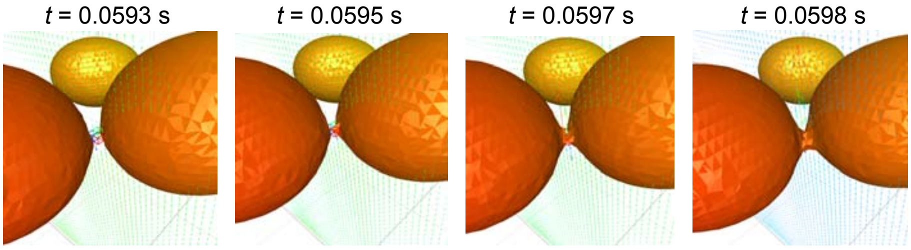
- Contribution of KIT (subcontractor of TU Hamburg Harburg): Development of improved turbulence models for bubbly flows using direct numerical simulations
  - A-priori testing of existing models and proposal of model improvements
  - A-posteriori testing by Euler-Euler simulations with OpenFOAM
  - Validation by experimental data for lab scale, pilot scale and industrial scale bubble columns
- Focus is on mono-disperse bubbly flows in organic liquids, Morton number M in range $10^{-7} – 10^{-10}$
- Status of PhD project of S. Erdogan (started in 2/2012)
  - d_B / d_{wall} = 1/4 – 1/6, Eötvös number in range 0.25 – 2.5
  - Grid independent results when bubble diameter is resolved by 20 cells
  - ρ_G/ρ_L = 1/25 gives results independent on ρ_G
  - Comparison with single bubble experiments of TUHH is underway
  - Problem: undesired coalescence in bubble swarm simulations

Coalescence: physical or not?

- $M = 10^{-8}$
- $d_B = 1\text{mm}$







$t = 0.0593$ s $t = 0.0595$ s $t = 0.0597$ s $t = 0.0598$ s

DNS methods and coalescence

- Front tracking methods (where the bubble is represented by a set of Lagrangian marker particles) suppress any coalescence unless a special merge condition is implemented
- Level-set methods and volume-of-fluid methods tend to merge bubbles automatically (and possibly unphysical) until a special prevention algorithm is implemented (e.g. representing each bubble by a own volume-fraction field)
- ⇒ all current methods are not predictive regarding coalescence
- To judge whether coalescence in numerical simulations are physical or not, well designed experiments for bubbles in pure systems would be useful which indicate the maximum bubble diameter where no coalescence occurs

Conclusions

- Flows in bubble columns are characterized by an inherent non-linear interaction between bubble-induced and shear-induced turbulence which is physically not fully understood
- One of the weakest points in Euler-Euler CFD computations of bubbly flows concerns adequate closures for turbulence
- Adapted single-phase two-equations models can provide reasonable results for the mean flow but not for turbulence quantities
  - Turbulence quantities are essential for predicting bubble size distribution
- DNS for insight (e.g. in the budget of k_L) and a-priori testing of closures
  - Modeling of interfacial term as work of drag force ✓
  - Closures for shear production and diffusive transport fail
  - Problem of reliably handling coalescence phenomena
- Combined theoretical, experimental and numerical efforts by the community are required to develop physically sound and general turbulence models for bubble-driven flows

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Acknowledgement

- Dr. M. Ilić (from Serbia)
- M.Sc. S. Erdogan

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