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Insights in liquid phase pseudo-turbulence and its transport equation by DNS of bubble swarms

"Multi-Phase" Project

BMBF-Network project (FKZ: 033RC1102H)

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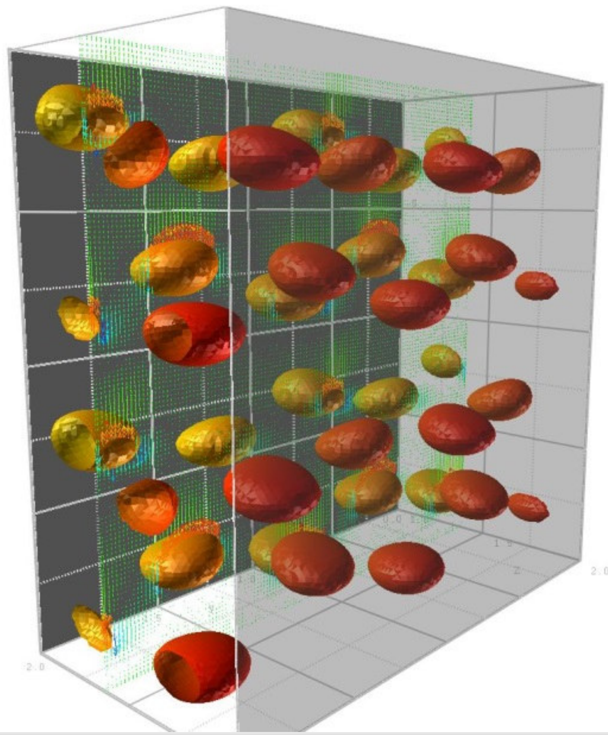
EVONIK INDUSTRIES

Sercan Erdogan, Martin Wörner

Jahrestreffen der ProcessNet „Mehrphasenströmungen"

March 24-25, 2014

Esperanto Hotel, Fulda



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- Introduction
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  - Evaluation of models for closure terms
- Conclusion and Outlook

Flow features and turbulence in bubble columns

Rising bubbles

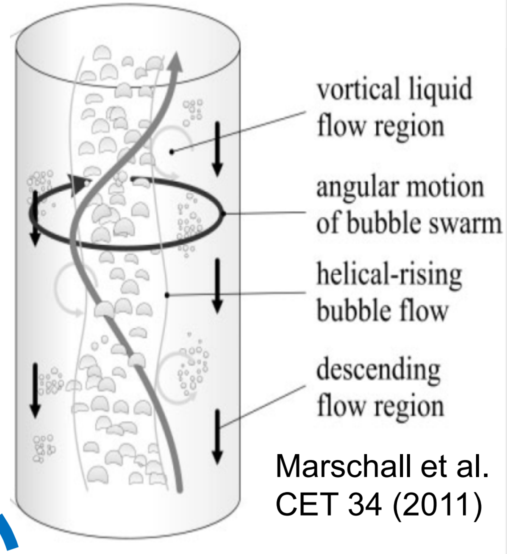
by displacement of liquid

Recirculating liquid flow
(upward in center, downward near wall)

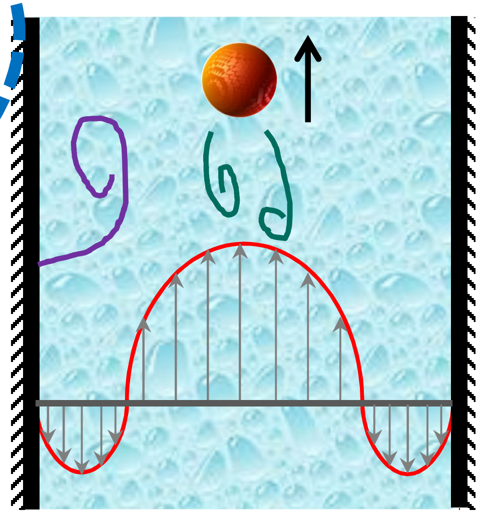
Shear-induced turbulence (SIT)
(especially near the walls)

Bubble-induced turbulence
(pseudo-turbulence) (BIT)

Inherent non-linear interaction
between BIT and SIT



Marschall et al.
CET 34 (2011)



Neither pure pseudo-turbulence is fully understood nor its interaction with shear-induced turbulence!

BMBF project Multiphase

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

The design approaches are limited for increasing the reactor performance → *May be useful* → *CFD methods* — *not yet used as tool for design of industrial scale bubble columns*

- Experience
- Empirical correlations
- Compartment models

Literature ↓

Euler-Euler approach based on Reynolds-averaged Navier-Stokes equations is the only approach that can meet industrial demands

k-ε models are reasonable approaches for predictions of the mean flow and TKE

TKE: Turbulence kinetic energy

Methodology

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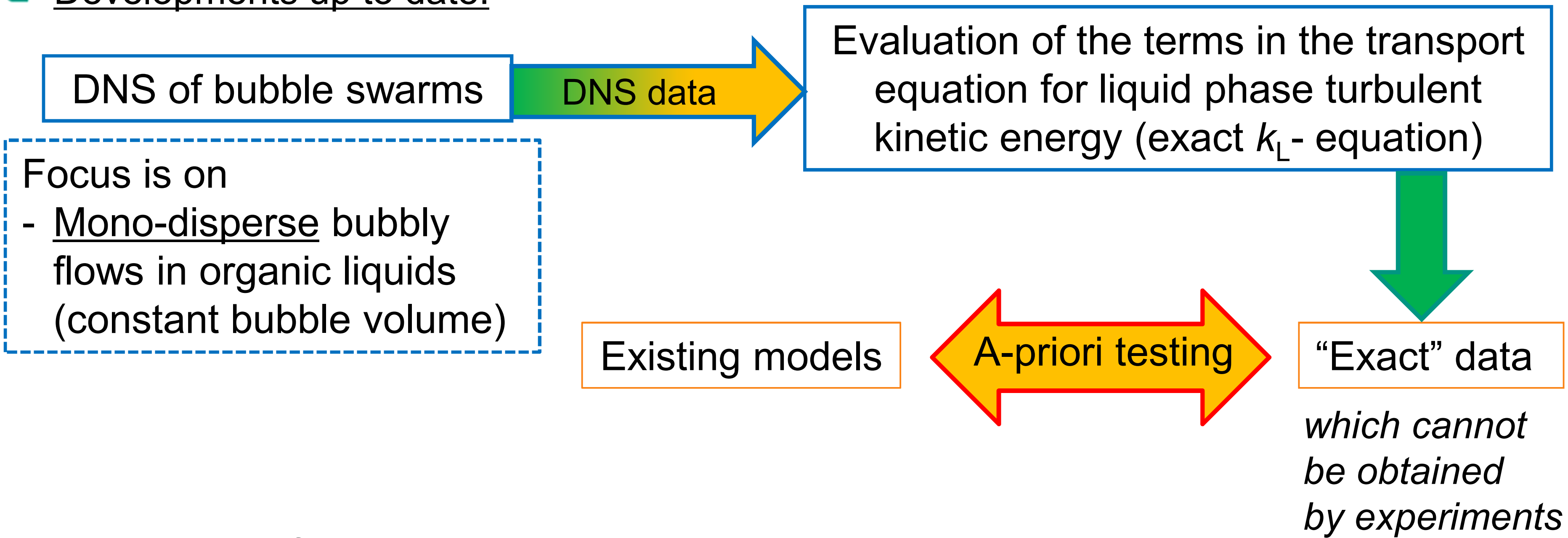
Contribution of KIT in BMBF project:

Goal: Development of improved turbulence models for bubbly flows by using DNS

- Developments up to date:



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

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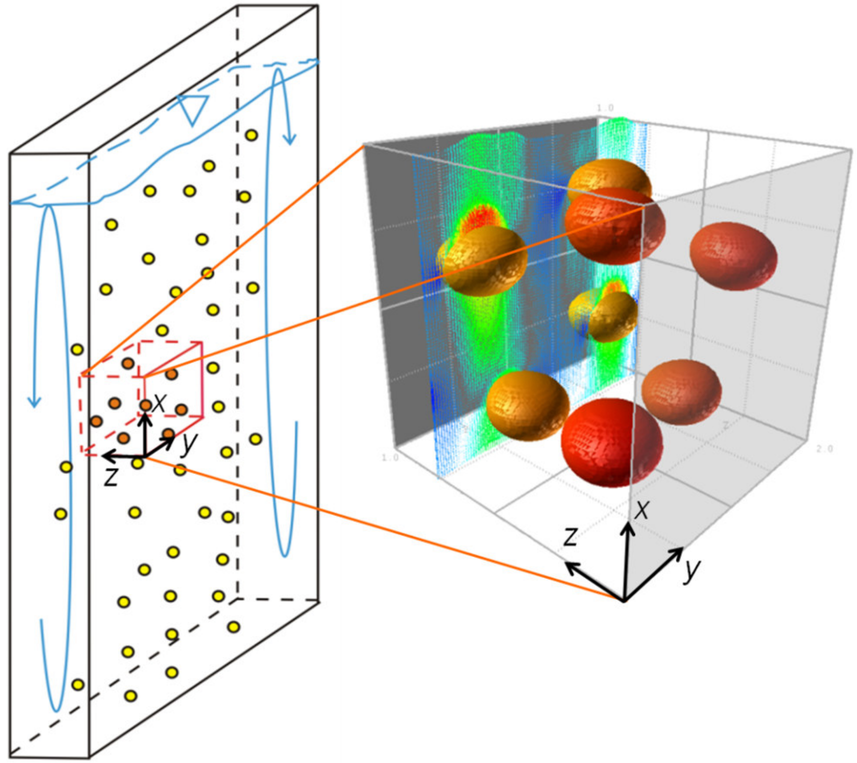
Set-up in our DNS studies

- Computational domain
  - Part of a flat bubble column
  - Two lateral side walls (*z*-direction)
    and periodic boundary conditions in vertical and transverse direction
    (*x*- and *y*-direction)
- Computer code (in-house)
  - Incompressible Navier-Stokes eqs. in single-field formulation
  - Volume-of-fluid method with piecewise linear interface reconstruction



- Why side walls are essential?
  - In triple-periodic domains the liquid recirculation typical for bubble columns is absent and production of TKE and dissipation are in local equilibrium
  - In wall-bounded flows there is usually no local equilibrium and TKE is redistributed by diffusion

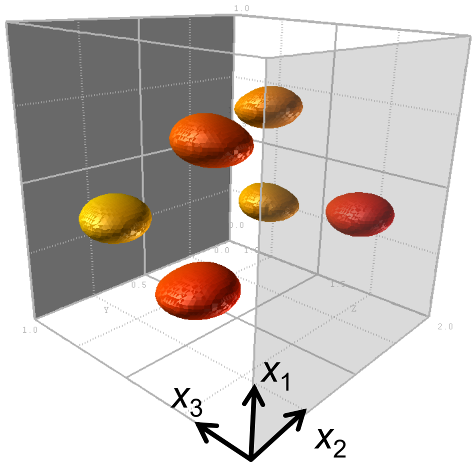
Set-up in our DNS studies

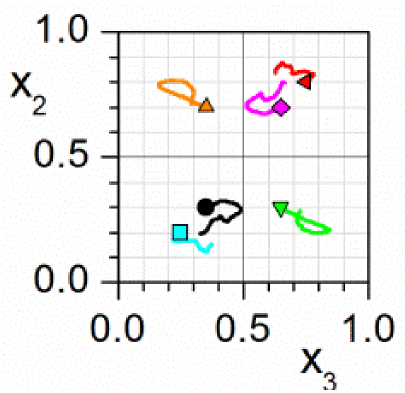
- PhD Thesis M. Ilic (2006)
  - Eötvös number = 3.065
  - Morton number *M,* in range $10^{-2} - 10^{-6}$
  - Up to 8 bubbles
  - Equidistant grid in wall direction

- Artificial wall contact
- The liquid film between the bubble and the wall is well resolved

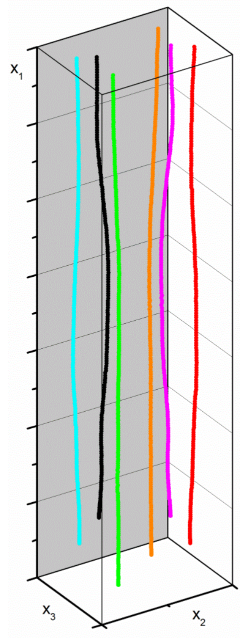
- Study is now extended to
  - Eötvös number in range 0.25 – 2.5
  - Morton number *M,* in range $10^{-7} - 10^{-10}$
  - Larger number of bubbles
  - Non-equidistant grid in wall direction with finer grid near the side walls

Bubble trajectories

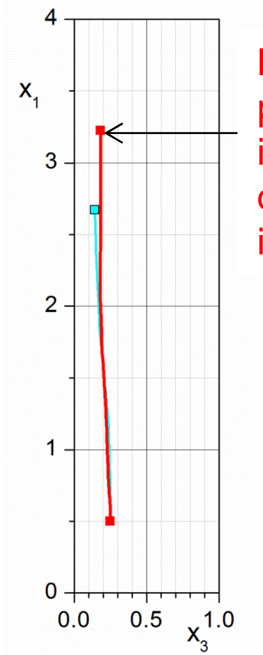




Above



Wall direction



Bubble position in wall direction is steady

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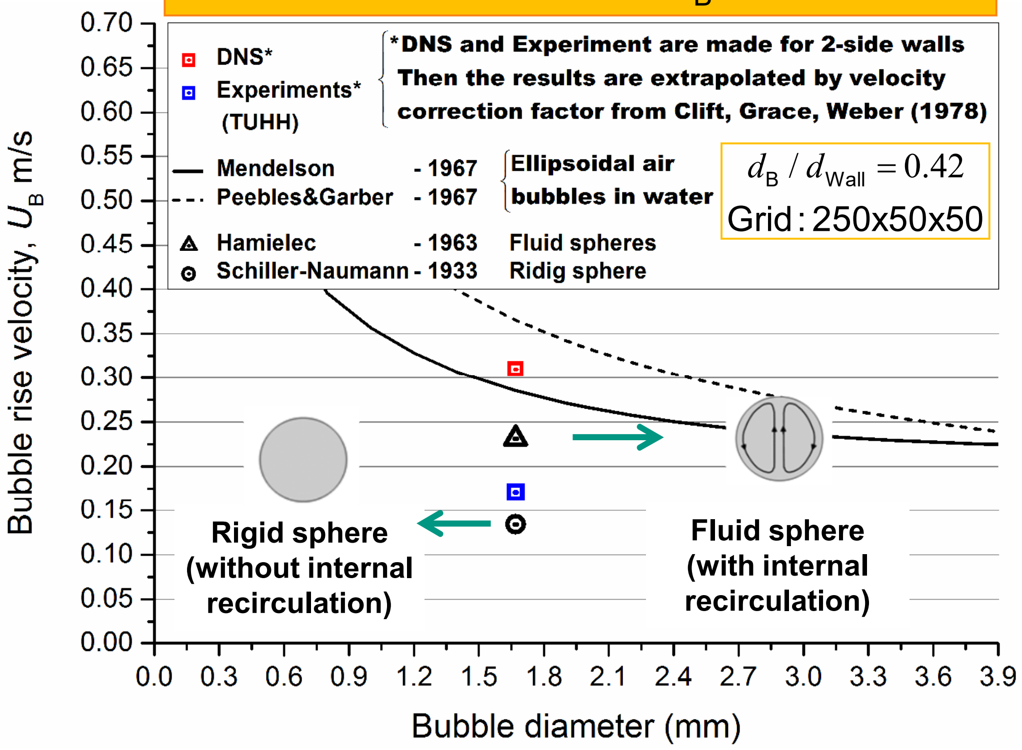
Single bubble simulations for validation

- Grid independent results when bubble diameter is resolved by about 20 cells
- ρ_G / ρ_L = 1/25 gives results independent from ρ_G

Water (%50) - Glycerin (%50) / Nitrogene
M=3.5x10^{-8} Eö=0.432 d_B=1.67 mm

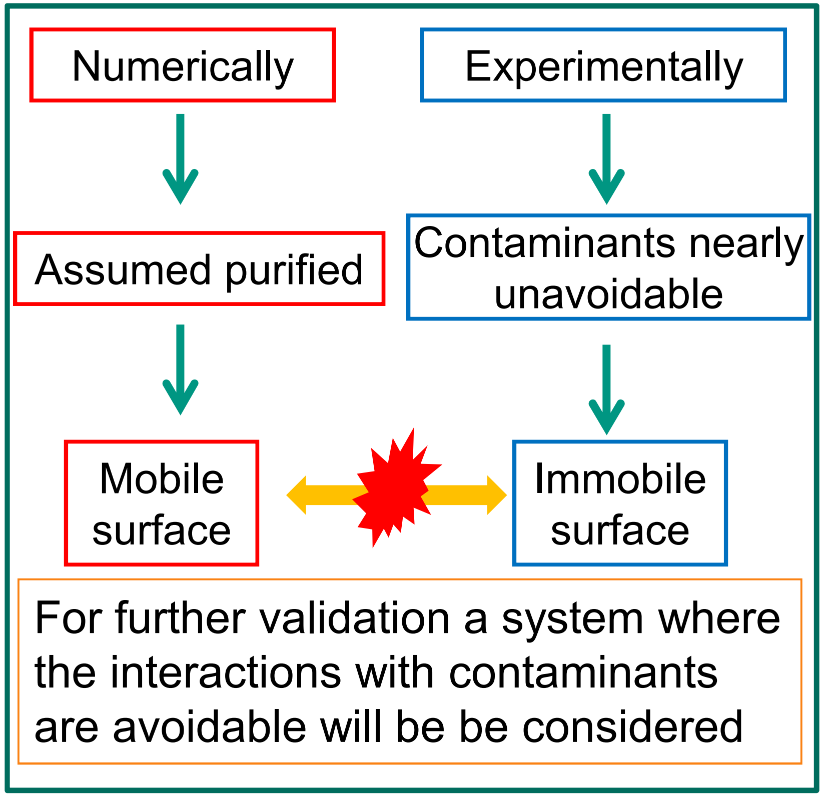


Bubble figures: Bothe M., Schlüter M., CET 85 (2013)

- The retarding effect of column walls on the terminal velocity of bubbles*

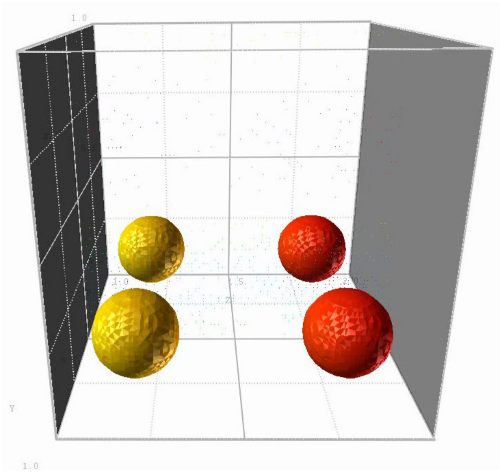
$$U_T / U_{T\infty} \approx 0.54$$

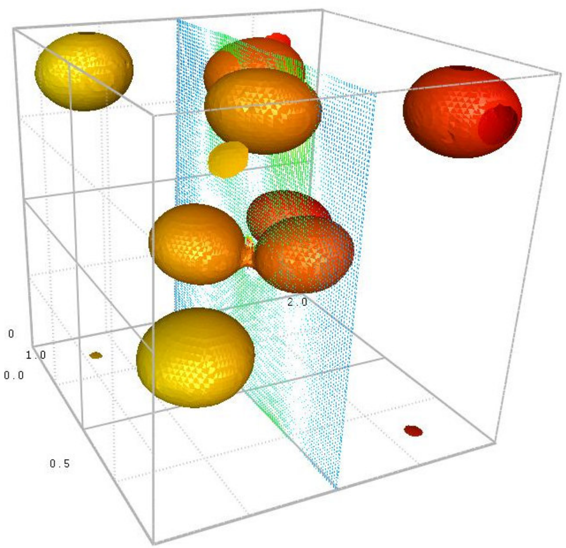
Direct comparison with single bubble experiments of TUHH is difficult



DNS of bubble swarms: Coalescence

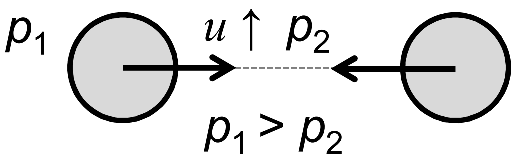
- $M = 10^{-8}$, d_B = 1mm

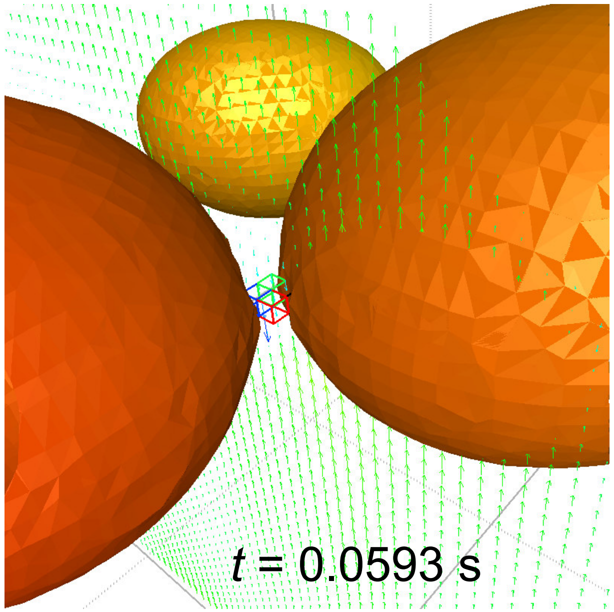




Between two bubbbles

$$u \uparrow \; \Rightarrow \; p \downarrow$$





- Bubble clustering
- Separating distances
- Gas holdup (ε)
  - d_B/d_{Wall}
  - Bubble diameter
  - Number of bubbles
- Coalescence may occur when $\varepsilon > 3\%$
- Lower void fraction is considered

$\varepsilon < 3\%$

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Simulation strategy

ε_1 **Small domain** → *statistically in steady state*

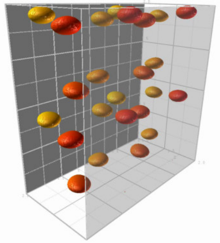
Replicated in the directions of periodic b.c.

Field $\{i, j, k\}$ → Field $\{(2i),(2j),k\}$

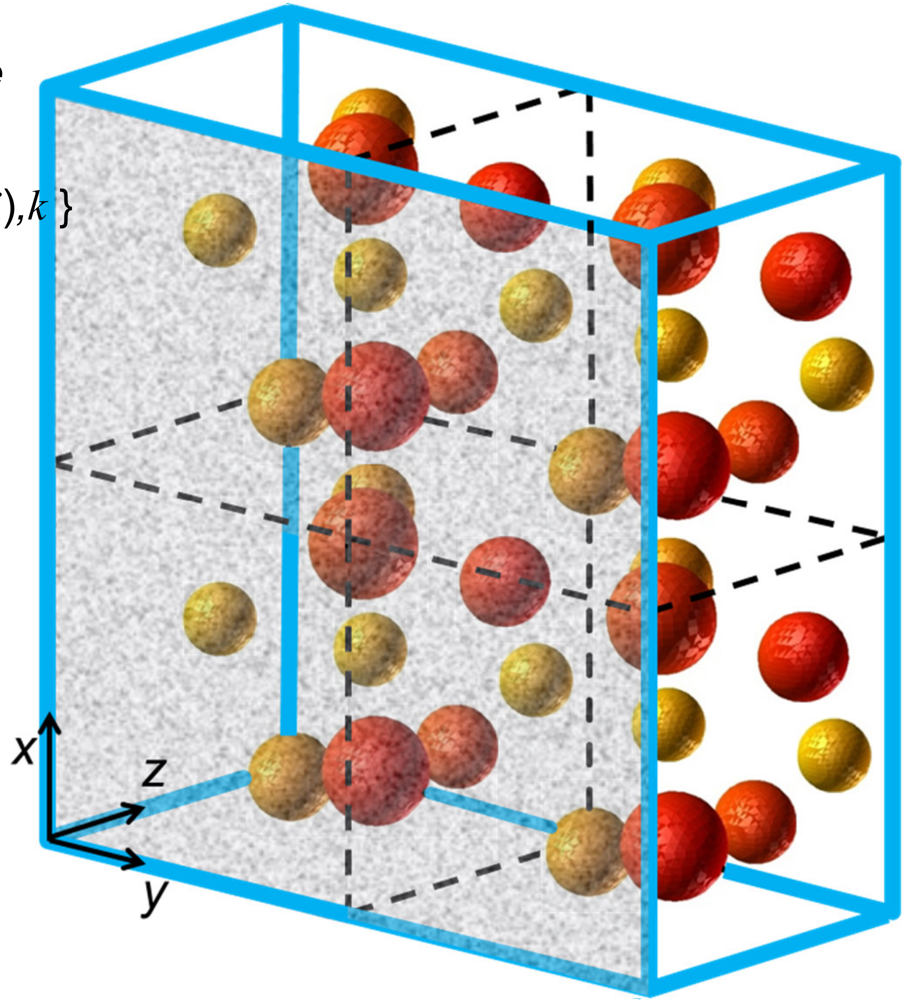
ε_2 **Larger domain**

- The same gas content $\varepsilon_1 = \varepsilon_2$
- Four times more number of bubbles

Simulation is continued



Bubble may re-order in the domain and have larger degree of freedom



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Exact analytical k_L equation

- k_L equation consists of single-phase-like terms and interfacial term
- Single-phase-like terms are in the same form as in the turb. kin. energy eq. for single phase flows (except being multiplied with the void fraction (α_L)

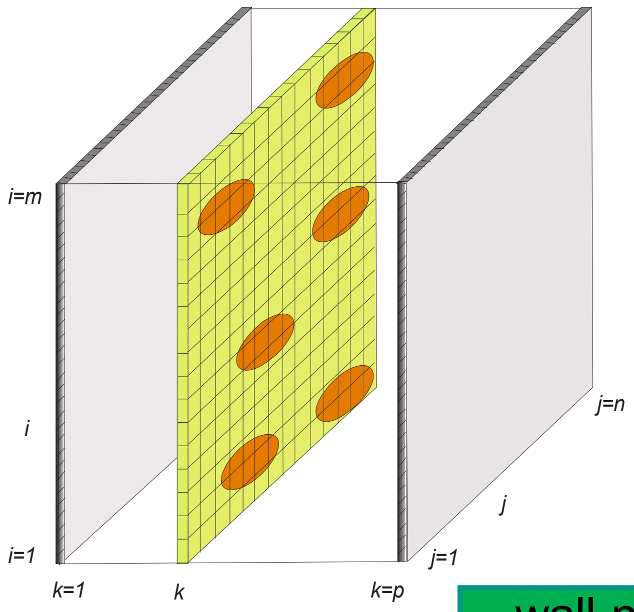
$$\frac{\partial}{\partial t}(\alpha_L k_L) + \nabla \cdot \left(\alpha_L k_L \overline{\overline{\mathbf{u}_L}}\right) = \underbrace{\frac{1}{Re_{ref}} \nabla \cdot \left(\alpha_L \overline{\overline{\tau_L^{'} \cdot \mathbf{u}_L^{'}}}\right) - \nabla \cdot \left[\alpha_L \left(\overline{\overline{p_L^{'} \mathbf{u}_L^{'}}} + \frac{1}{2} \overline{\overline{\mathbf{u}_L^{'2} \mathbf{u}_L^{'}}}\right)\right]}_{DIFFUSION}$$

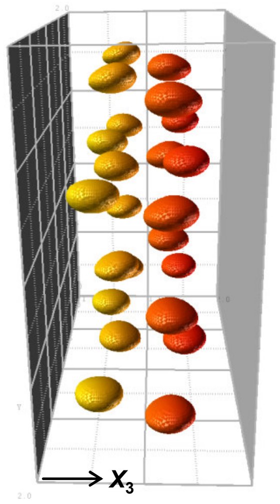
$$\underbrace{-\alpha_L \overline{\overline{\mathbf{u}_L^{'} \mathbf{u}_L^{'}}} : \nabla \overline{\overline{\mathbf{u}_L}}}_{PRODUCTION\ BY\ SHEAR} \underbrace{- \frac{1}{Re_{ref}} \alpha_L \overline{\overline{\tau_L^{'} : \nabla \mathbf{u}_L^{'}}}}_{DISSIPATION} + \underbrace{\overline{\left[\frac{1}{Re_{ref}} \tau_{L,i}^{'} - p_{L,i}^{'} \mathbb{I}\right] \cdot \mathbf{u}_{L,i}^{'} \cdot \hat{\mathbf{n}}_{L,i} a_i}}_{PRODUCTION\ BY\ INTERFACIAL\ TERM}$$

Kataoka & Serizawa (1989)

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

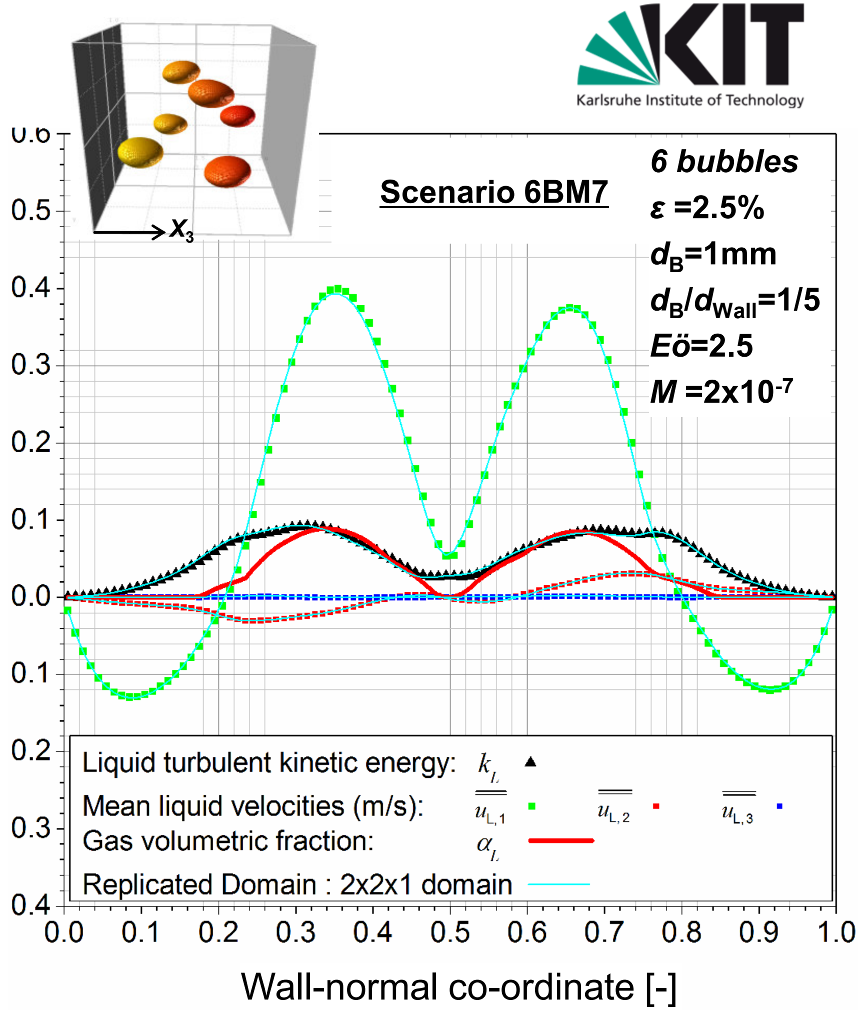
Averaging of simulation results





$$\overline{\overline{u}}_{L,3} \approx 0$$

wall normal profiles



- Averaging over planes parallel to the side walls (within fully developed regime)
- Additional averaging over different instants in time

- Profiles are not fully symmetrical → Larger averaging period is required
- Results for replicated domains are similar

Quantitive analysis: Budget of basic k_L equation

- k_L equation is calculated using the DNS data

$$\underbrace{\frac{\partial}{\partial t}\left(\alpha_L k_L\right)+\nabla\cdot\left(\alpha_L k_L \overline{\overline{\mathbf{u}_L}}\right)=}$$

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

$$\underbrace{-\alpha_L\overline{\overline{\mathbf{u}'_L\mathbf{u}'_L}}:\nabla\overline{\overline{\mathbf{u}_L}}}_{PRODUCTION}$$

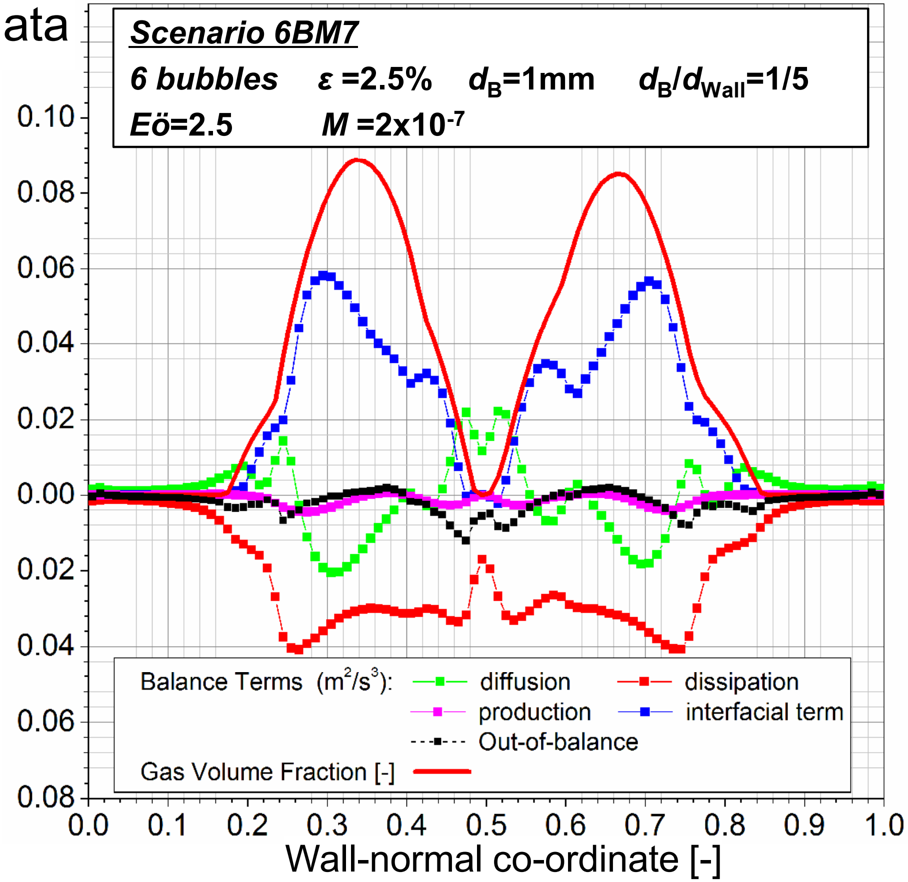
Negligible

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

No local equilibrium

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

Main source term



- Out of balance term is around 5% of the total production
- Interfacial term is main source (production by shear is negligible here)
- No local equilibrium between total production and dissipation
- Redistribution of TKE from high void fraction to low void fraction region by diffusion

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Diffusion term

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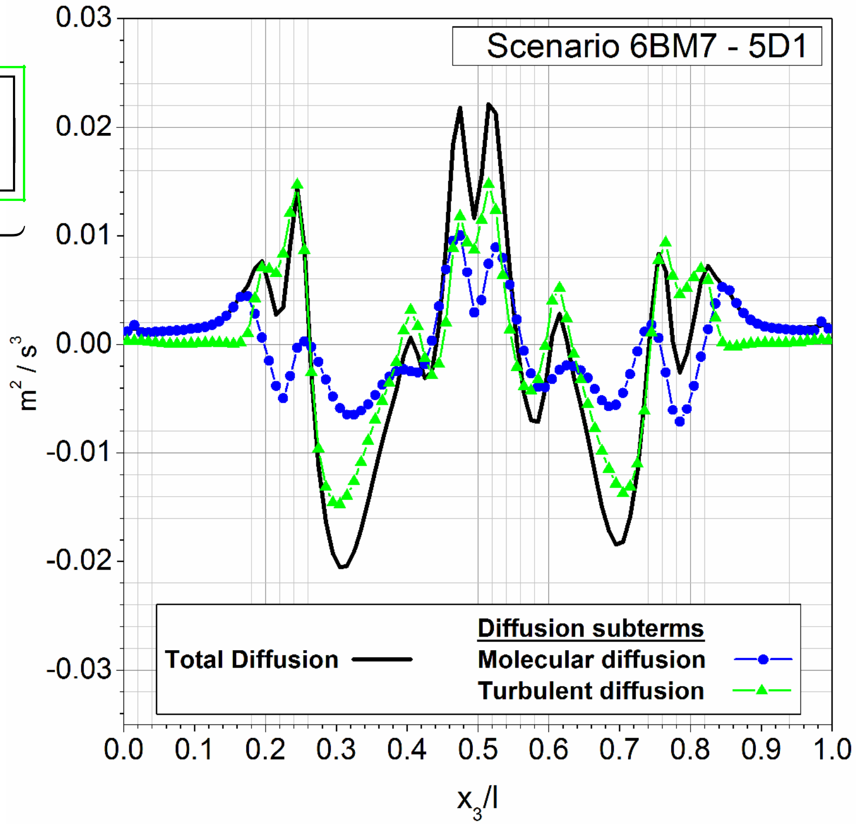
- Diffusion term is important → Employed for transport of TKE

Molecular Diff. — Turbulent Diff.

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

Fluctuating liquid pressure gradient (Pressure correlation)

Fluctuating velocity (Triple correlation)



- Turbulent diffusion:
  - The main part of total diffusion
  - It cannot be measured → must be modelled

- Modelling of diffusion term is difficult due to its complex profiles
- Standard single-phase type models have poor performance (strongly underestimate the diffusion term)

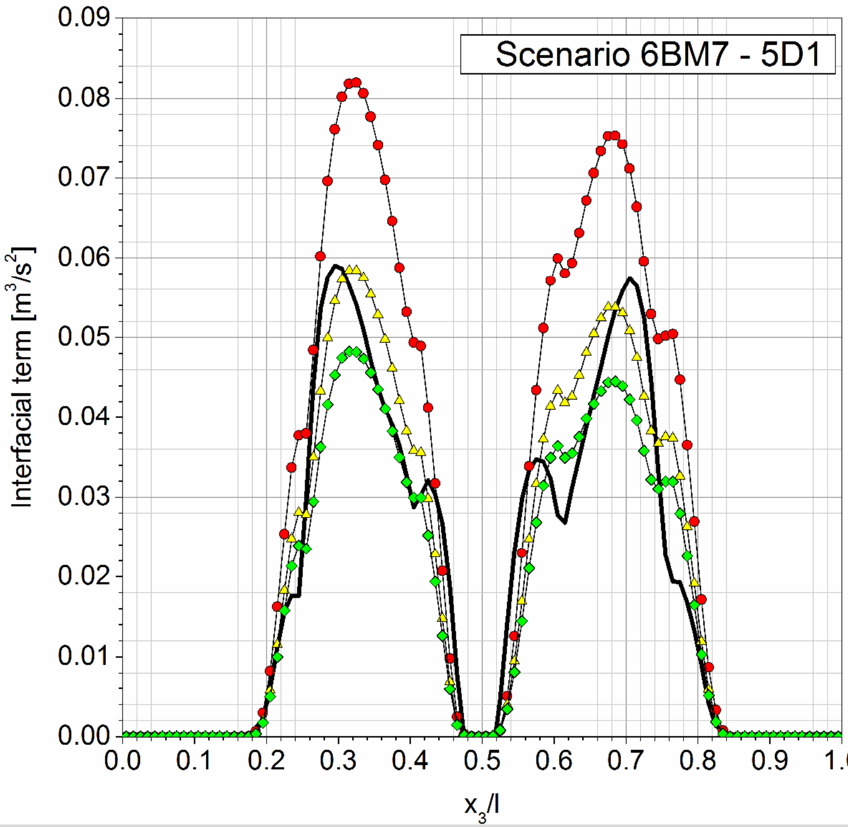
Interfacial term

- Comparing to other balance terms it is the most complex one (12 sub-terms)
- Directly related to the presence of bubble interfaces
- Main source of the liquid turbulence kinetic energy in the present case

—— *"exact" interfacial term by using DNS data*: $-\overline{p'_{L,in} u'_{Li,in} n_{Li} a_{in}} + \overline{\tau'_{Lij,in} u'_{Li,in} n_{Lj} a_{in}}$

CLOSURE ASSUMPTIONS	
Drag contribution defined by mean quantities	**Model**
Including drag force $W_D = 0.75 C_D \alpha_G \rho_L \left|\overline{\overline{\mathbf{u}_r}}\right|^3 / d_B$ With non-drag contribution $F_{am} \overline{\overline{\mathbf{u}_r}}$ (with added mass force)	**Morel**
Partly including the drag force $0.75 W_D$	**Olmos et al.**
Drag force not explicitly included $0.25 \alpha_L \alpha_G \rho_L \left(1 + C_D^{4/3}\right) \left|\overline{\overline{\mathbf{u}_r}}\right|^3 / d_B$	**Lahey et al.**

***C_D* → Drag coefficient (different formulations used)**



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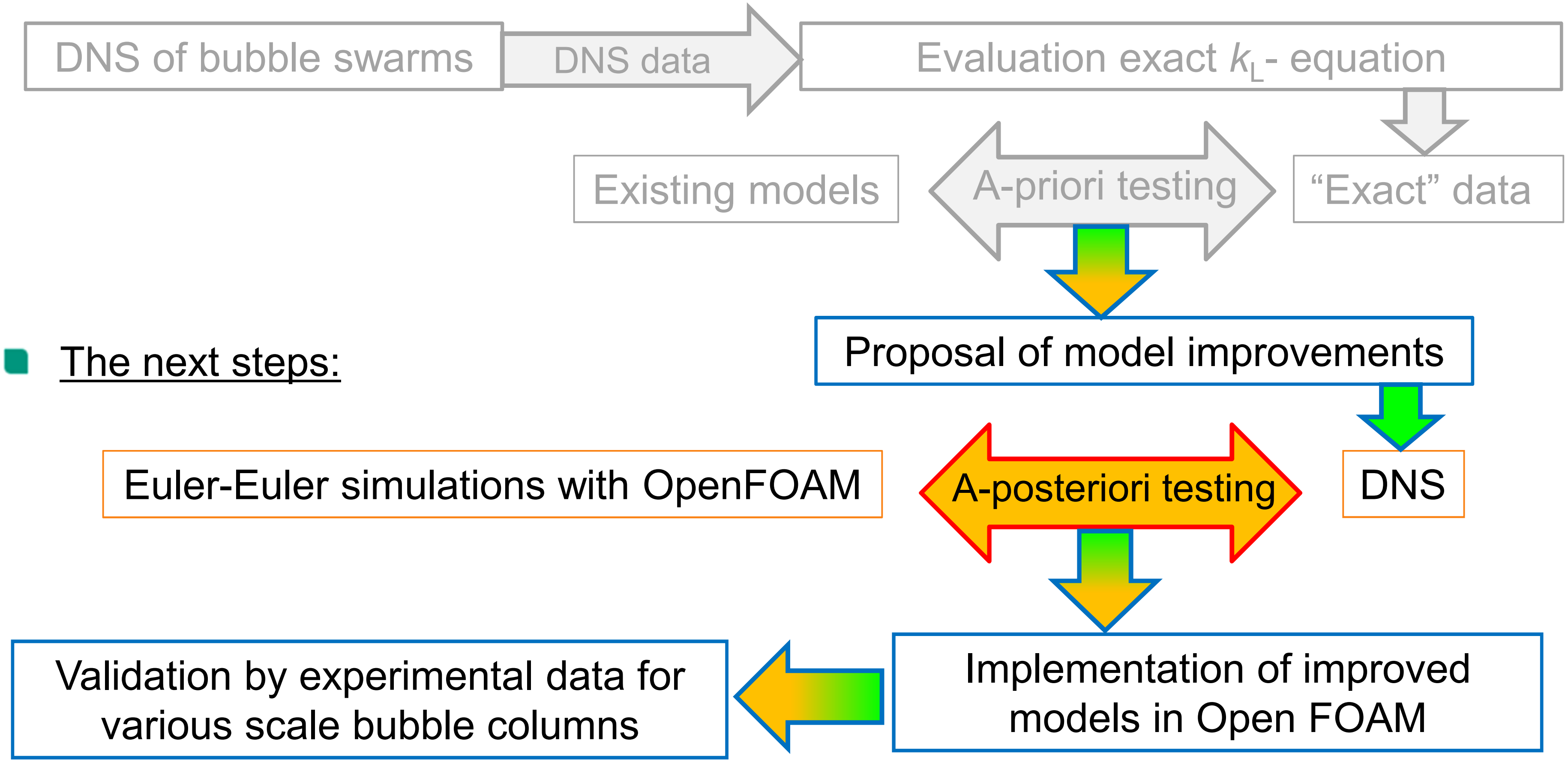
Conclusion

- Up to now Morton number $M = 10^{-7}$ and 10^{-8} are considered
- $M < 10^{-8}$ up to 10^{-10} for different *Eö* and d_B / d_{wall} should be considered
  - Eötvös number in range 0.25 – 2.5
  - $d_B / d_{wall} = 1/4 – 1/6$
- The result for analysis of liquid phase turbulent kinetic energy are consistent
  - With replication technique, domain size is sufficiently large and statistical data are independent of domain size
  - Out of balance is sufficiently small $\rightarrow$ statistical data are reliable
  - Development of improved models for significant closure terms (diffusion and interfacial production) in the k_L equation is ongoing

Outlook

- <u>The next steps:</u>



- <u>A-posteriori testing of Euler-Euler simulations with OpenFOAM:</u>

  Assessment of the potential non-linear interaction between models for bubble forces, bubble size distribution and turbulence in engineering CFD computations

- This work is sponsored by the German Federal Ministry of Education and Research (01RC1102)
- **Information on *"Multi-Phase" Project* :**

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Campus Blasensäulen July, 2013

Volume 85, Issue 7 Pages 965–1155

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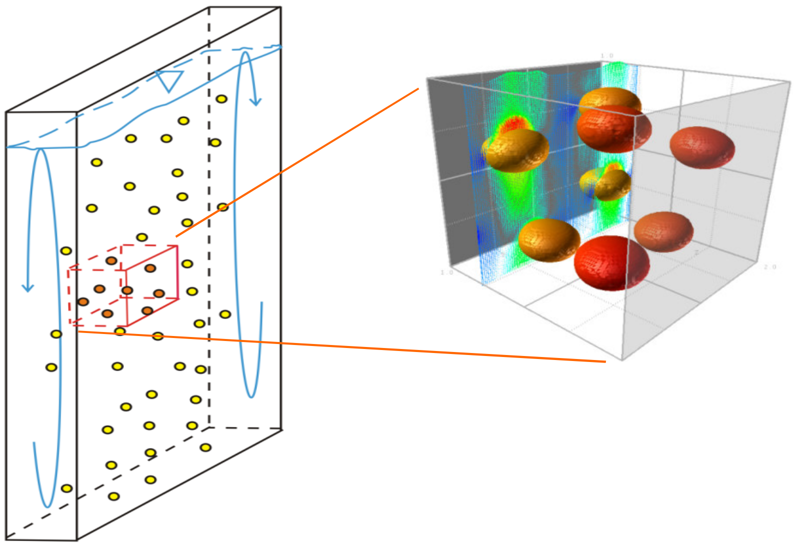

Thank you for your attention...