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Volume-of-fluid method based numerical simulations of gas-liquid flow in confined geometries

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Merits of DNS of gas-liquid flow

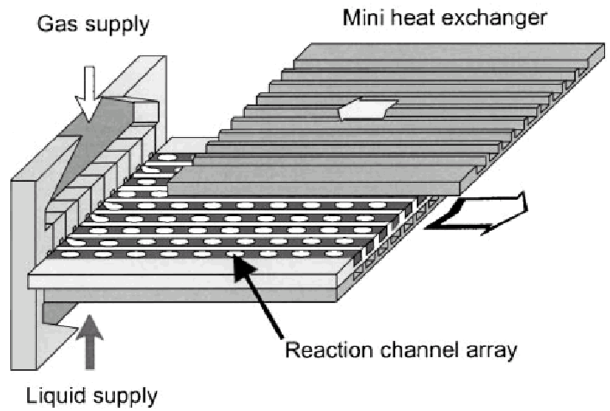
- Allows to get deeper insight into flow mechanisms and thus fosters physical understanding
  - Here: bubble train flow in square mini-channel
- Provides a complete database of the 3D velocity and pressure field and phase distribution with high spatial and temporal resolution
  - Here: analysis of liquid phase turbulence kinetic energy equation for bubble swarm flow

In-house code TURBIT-VOF

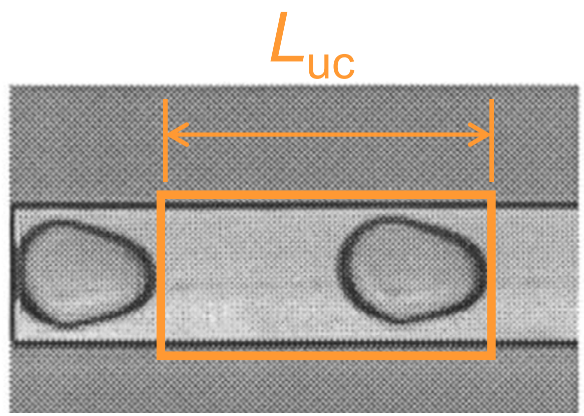
- Volume-of fluid method for interface tracking
  - Interface is locally approximated by plane (PLIC method)
- Governing equations for two incompressible fluids
  - Single field momentum equation with surface tension term
  - Zero divergence condition for center-of-mass velocity
  - Advection equation for liquid volumetric fraction *f*
- Solution strategy
  - Projection method resulting in pressure Poisson equation
  - Explicit third order Runge-Kutta time integration scheme
- Discretization in space
  - Finite volume formulation for regular staggered grid
  - Second order central difference approximations

Multi-phase micro process engineering

- Miniaturized devices offer certain advantages
  - High interfacial area per unit volume
    $\Rightarrow$ Enhanced heat and mass transfer
  - Defined interface geometry
    $\Rightarrow$ Numbering up instead of scaling up
  - Example: Micro bubble column*



- Flow pattern in single channel: bubble train flow
  - Bubbles of identical shape move with same velocity
  - Flow is fully characterized by a single "unit cell" of length L_{uc}



* Institute for Micro Technology, IMM, Mainz, Germany

Numerical set up

- Square vertical channel with cross section 2 mm $\times$ 2 mm
- Consideration of <u>one</u> flow unit cell only
- Account for influence of trailing/leading unit cells by <u>periodic boundary conditions</u> in axial direction
- Length of flow unit cell, L_{uc}, is input parameter
- Flow is driven in vertical direction (*y*) by specified axial pressure gradient and buoyancy

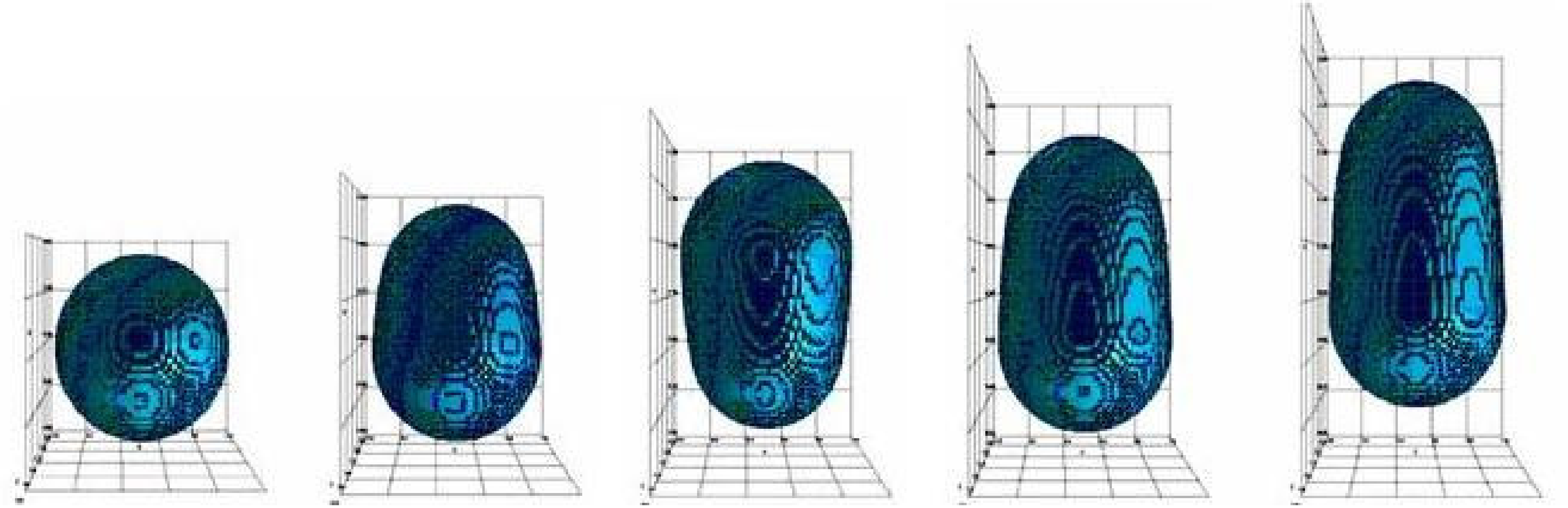
Physical parameters

- Fluid properties

Factor 10 higher than ρ and μ of air

ρ_l	ρ_g	μ_l	μ_g	σ
957 kg/m^3	11.7 kg/m^3	0.048 Pa s	1.84×10^{-4} Pa s	0.022 N/m

- Initial bubble shapes (void fraction ε = 33%)



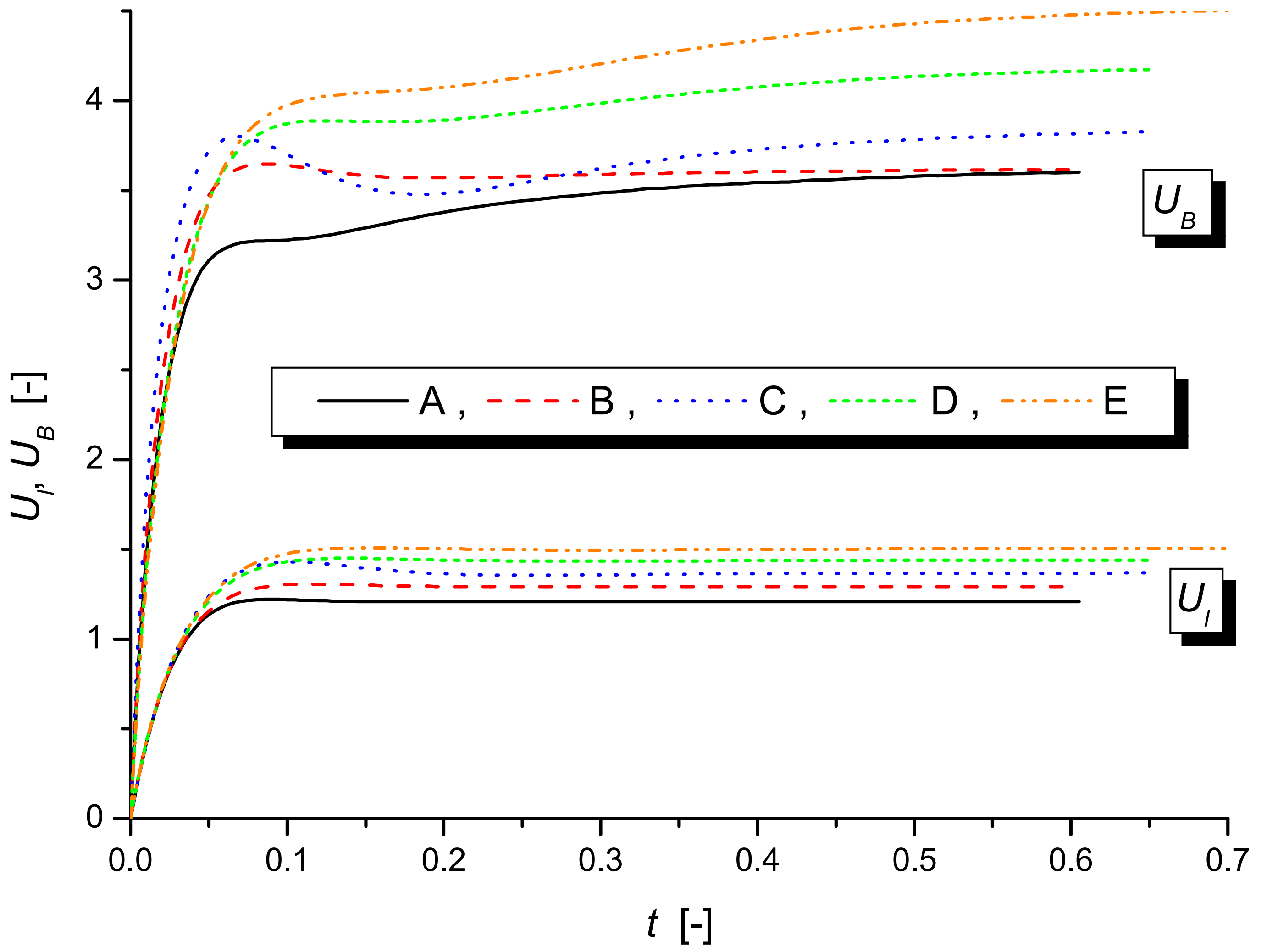
- Simulations are started from gas and liquid at rest

Computational parameters

Case	L_{uc} / W	Domain	Grid	Time steps
A1	1	$1 \times 1 \times 1$	$48 \times 48 \times 48$	24,000
A2	1	$1 \times 1 \times 1$	$64 \times 64 \times 64$	60,000
B	1.25	$1 \times 1.25 \times 1$	$48 \times 60 \times 48$	24,000
C	1.5	$1 \times 1.5 \times 1$	$48 \times 72 \times 48$	26,000
D	1.75	$1 \times 1.75 \times 1$	$48 \times 84 \times 48$	26,000
E	2	$1 \times 2 \times 1$	$48 \times 96 \times 48$	28,000

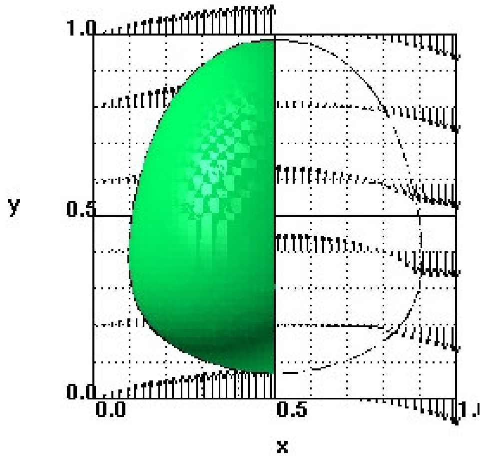
Results on both grids show only slight differences

Time history of mean velocities



Steady state values of bubble velocity U_B and mean liquid velocity U_l increase with increasing length of the flow unit cell

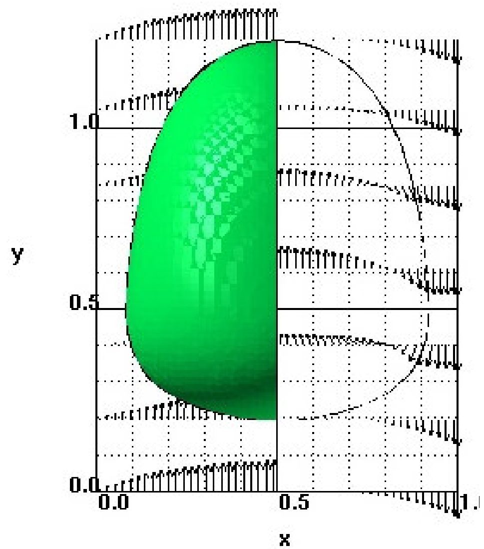
Bubble shape and velocity field

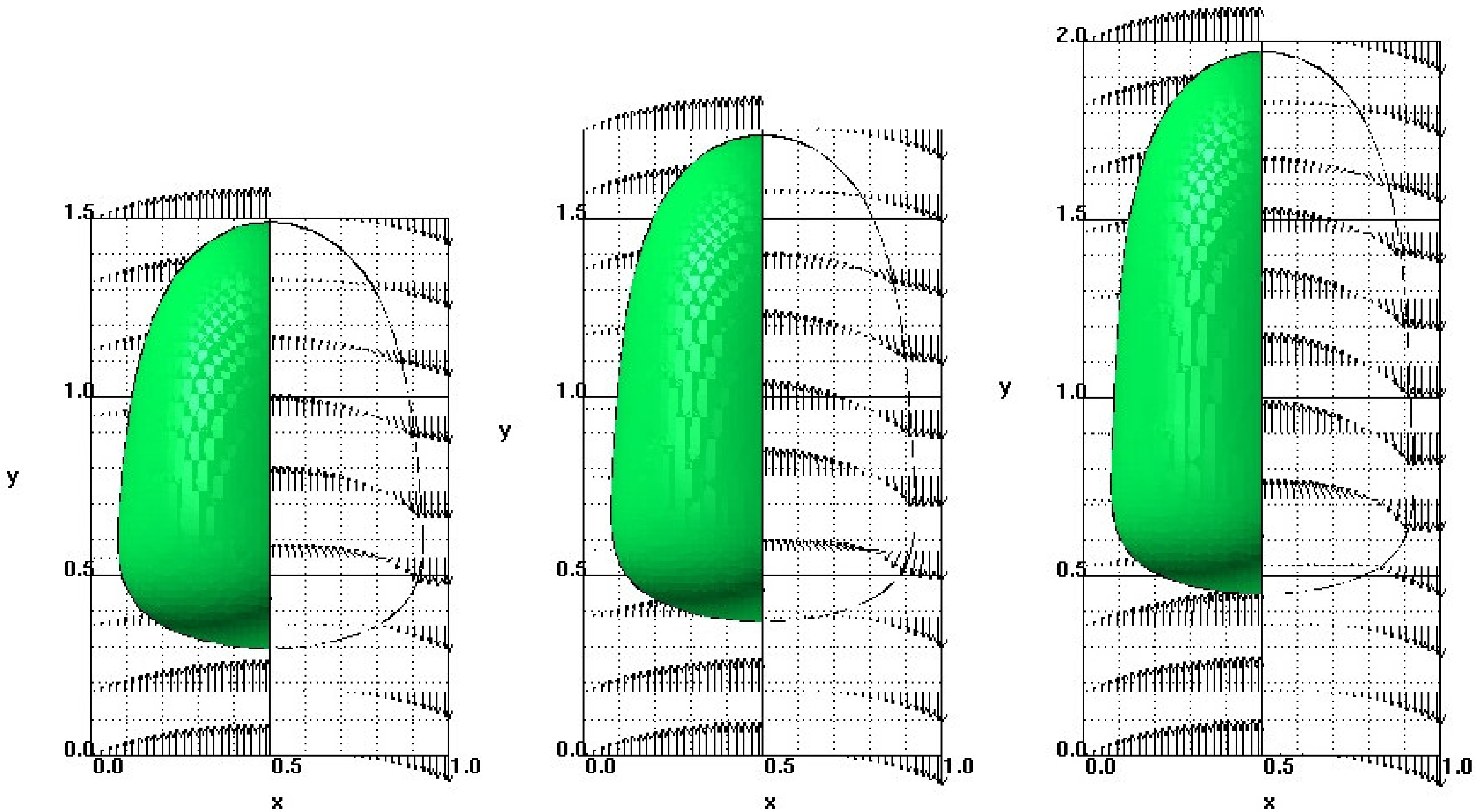


Velocity field in vertical mid-plane

Right half: frame of reference moving with bubble

Left half: fixed frame of reference



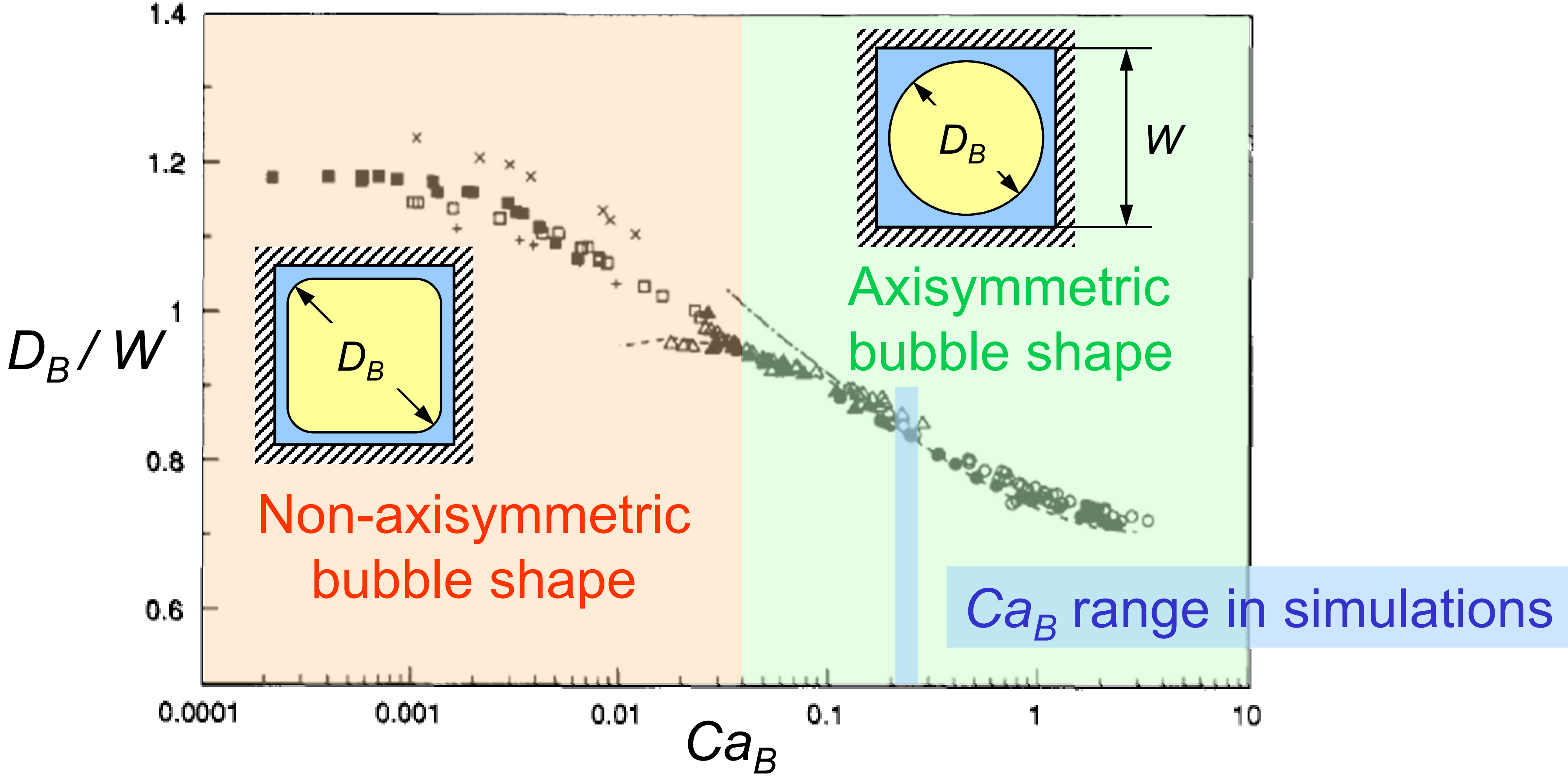


Comparison with experiment

Case	L_{uc} / W	Ca_B	D_B / W	$(U_B – J_{total})/U_B$	U_B/J_{total}
			Non-dimensional bubble diameter	Relative velocity	Non-dimensional U_B
A	1	0.204	0.81	1.80	0.445
B	1.25	0.207	0.84	1.75	0.430
C	1.5	0.215	0.85	1.75	0.430
D	1.75	0.238	0.85	1.78	0.438
E	2	0.253	0.85	1.8	0.445
Experimental data* correlated in terms of capillary number $Ca_B \equiv \mu_l U_B / \sigma$					
		0.2 – 0.25	0.82 – 0.86 ✓	1.68 – 1.84 ✓	0.435 – 0.475 ✓

* Thulasidas, Abraham, Cerro, Chem. Eng. Science 50 (1995) 183-199

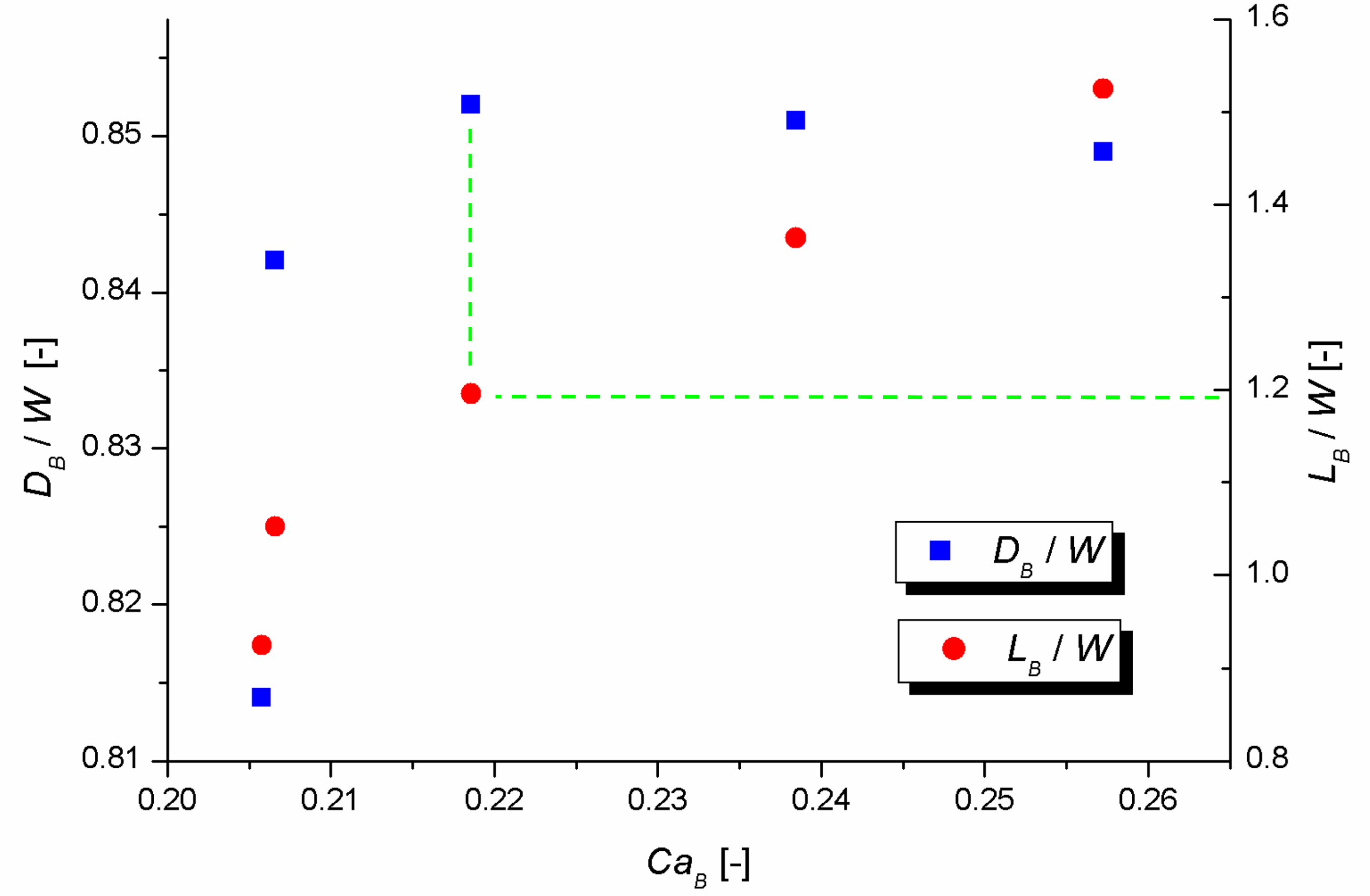
D_B measured along channel diagonal*



⇒ D_B / W decreases with increase of Ca_B

* Thulasidas, Abraham, Cerro, Chem. Eng. Science 50 (1995) 183-199

Bubble diameter in simulations



D_B / *W* decreases with increase of Ca_B <u>only</u> if the bubble length L_B is larger than about 1.2 the channel width (this is the case in the experiments by Thulasidas et al.)

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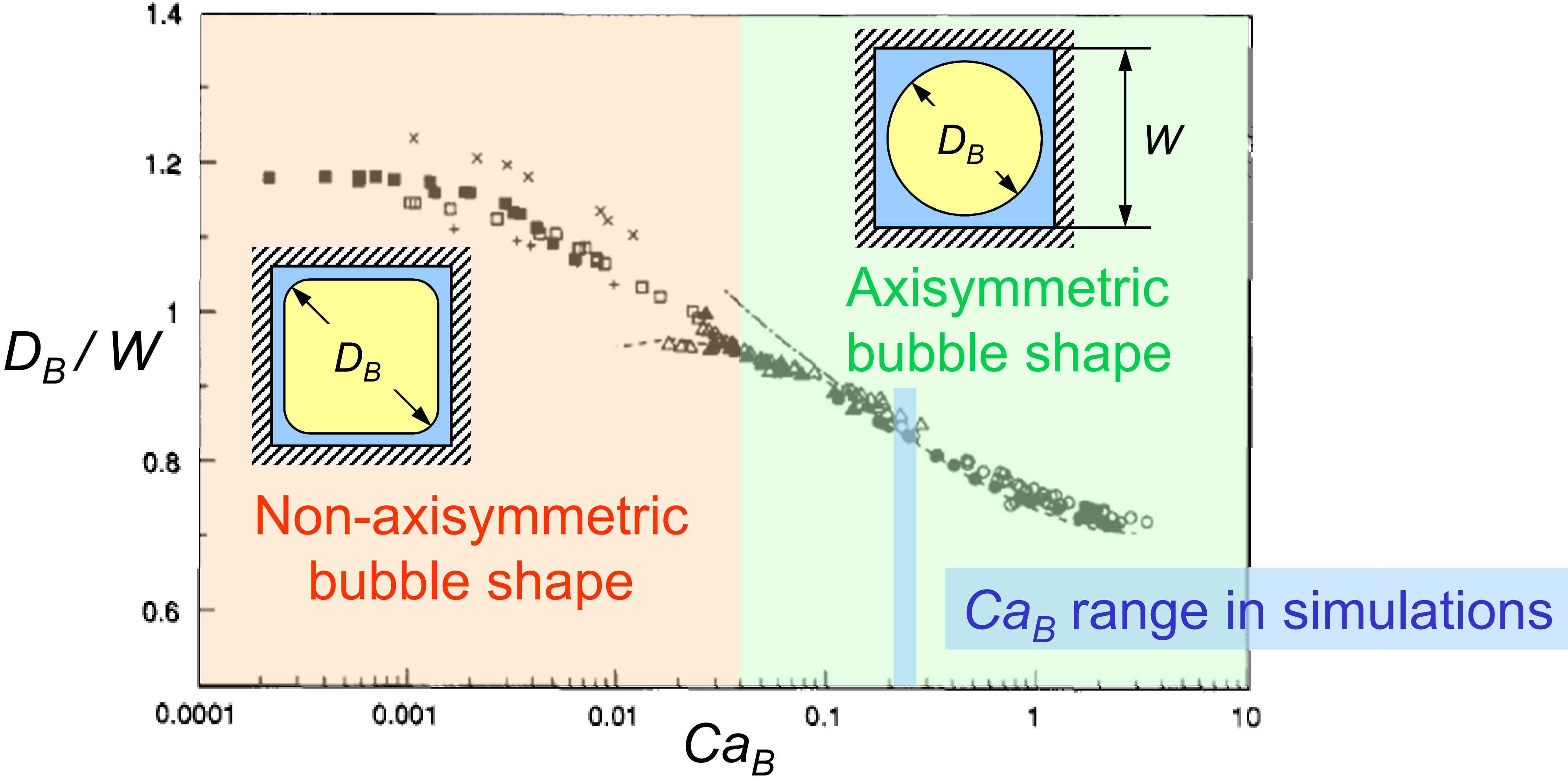
D_B measured along channel diagonal*



⇒ D_B / W decreases with increase of Ca_B

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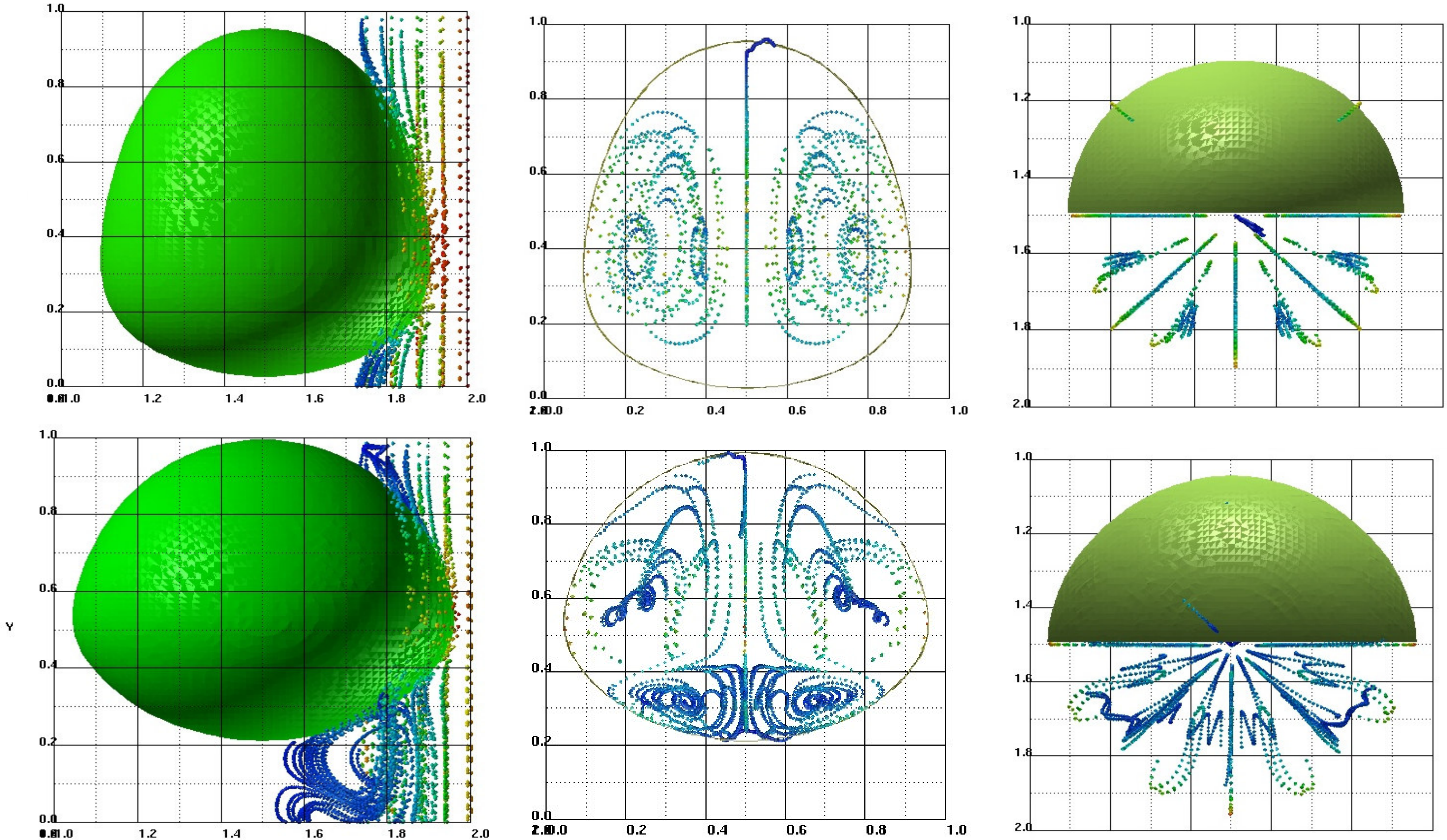
Influence of capillary number

top row: Ca = 0.205, bottom row: Ca = 0.043



Turbulence modeling for bubbly flow

- No generally accepted model available in literature
- Analytical turbulence kinetic energy eq. for liquid phase*:

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

$$\underbrace{-\alpha_L \overline{\overline{\mathbf{u}_L'\mathbf{u}_L'}} : \nabla\overline{\overline{\mathbf{u}_L}}}_{PRODUCTION} \underbrace{- \frac{1}{Re_{ref}}\alpha_L \overline{\overline{\mathbb{T}_L' : \nabla\mathbf{u}_L'}}}_{DISSIPATION} + \underbrace{\overline{\left[\frac{1}{Re_{ref}}\mathbb{T}_{L;in}' - p_{L;in}'\mathbb{I}\right]\cdot\mathbf{u}_{L;in}'\cdot\mathbf{n}_{L;in} a_{in}}}_{INTERFACIAL\ TERM}$$

$$k_L \equiv \frac{1}{2}\overline{\overline{\mathbf{u}_L'\cdot\mathbf{u}_L'}} = \frac{1}{2}\frac{1}{{U_{ref}^*}^2}\overline{\overline{\mathbf{u}_L^{*\prime}\cdot\mathbf{u}_L^{*\prime}}}$$

$$\mathbb{T}_L' = \mu_L\left[\nabla\mathbf{u}_L' + (\nabla\mathbf{u}_L')^T\right]$$

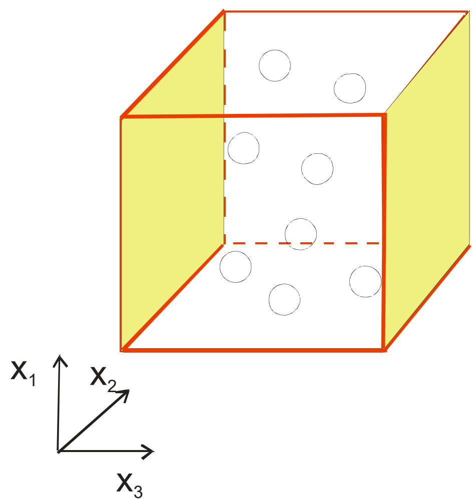
$$\overline{A_L} = \text{averaging} \qquad \overline{\overline{A_L}} = \overline{A_L X_L}/\overline{X_L} \qquad \alpha_L = \overline{X_L}$$

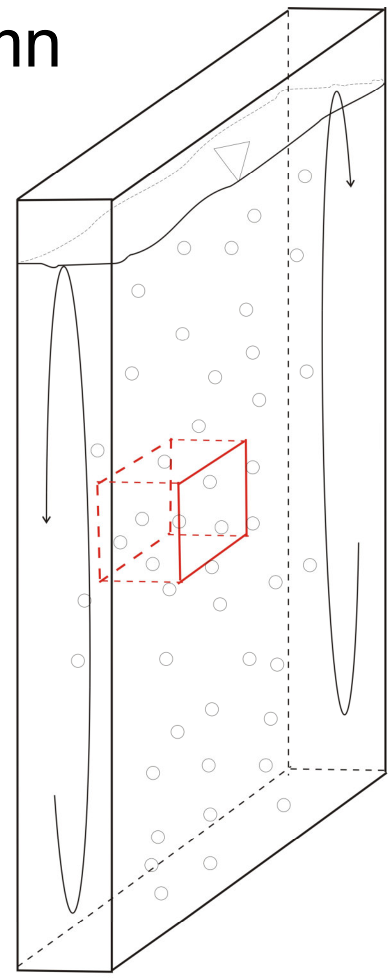
$$A_L' = A_L - \overline{\overline{A_L}} \qquad A_{Lin}' = A_{Lin} - \overline{\overline{A_L}}$$

*Kataoka & Serizawa (1989)

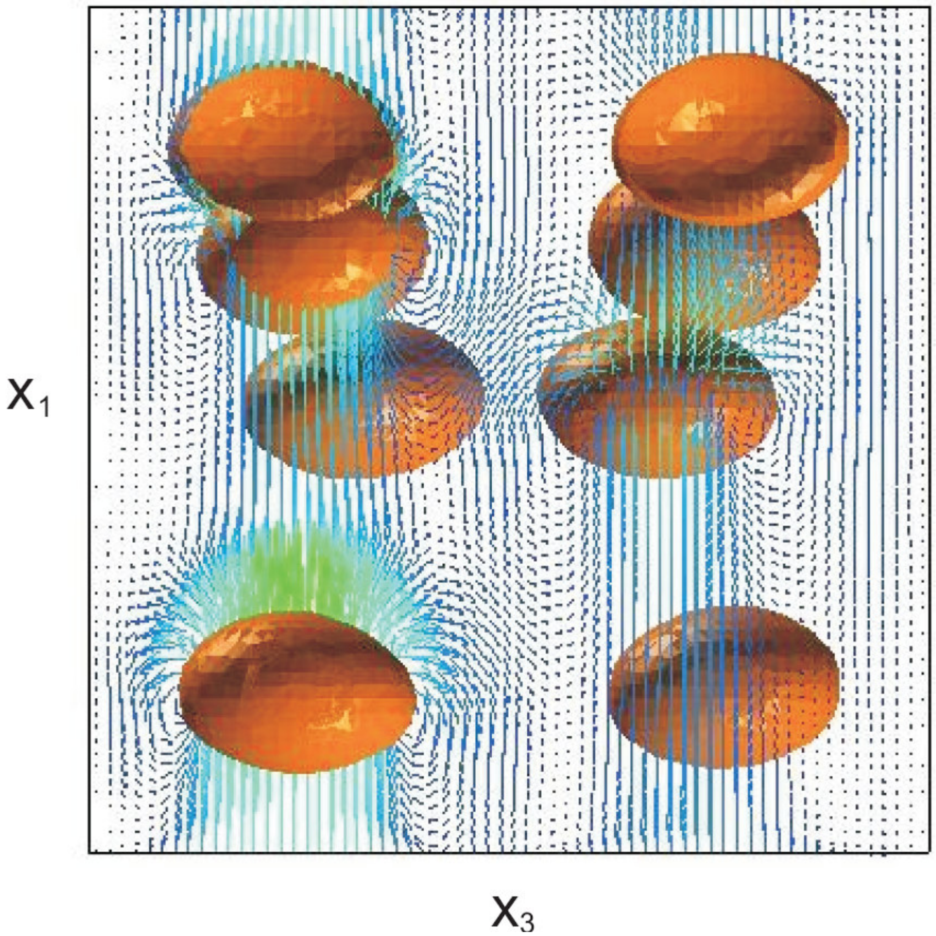
Simulation of bubble swarm flow

- Simulation mimics section of a flat bubble column
  - periodic b.c. in vertical and span-wise directions
  - rigid lateral walls
- Domain: 1 × 1 × 1, Grid: 64 × 64 × 64
- Eight bubbles with $d_B/W = 0.25$ ($\varepsilon = 6.5\%$)
- Phase density ratio: 0.5
- Phase viscosity ratio: 1
- Bubble Eötvös number: 3.065
- Morton number: $3.06 \cdot 10^{-6}$

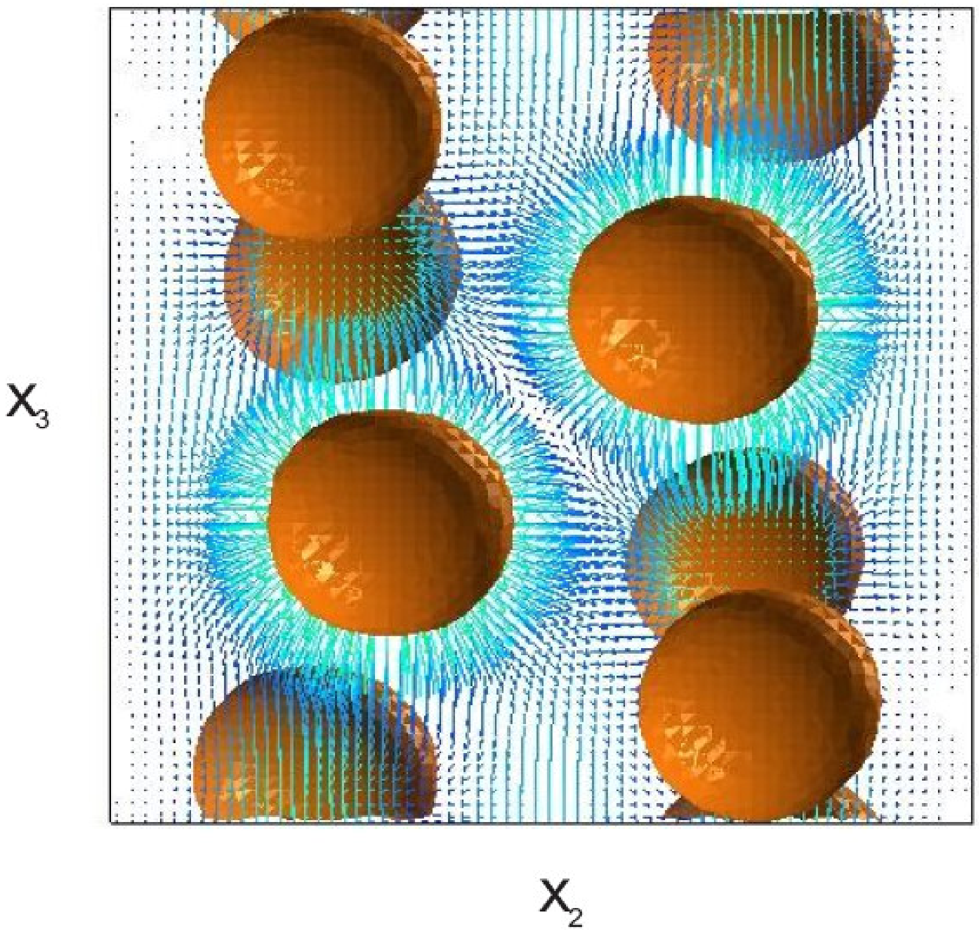




Flow visualization



view from side



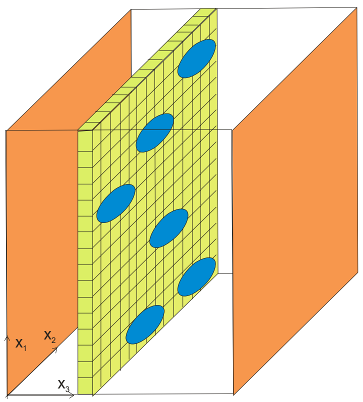
view from top

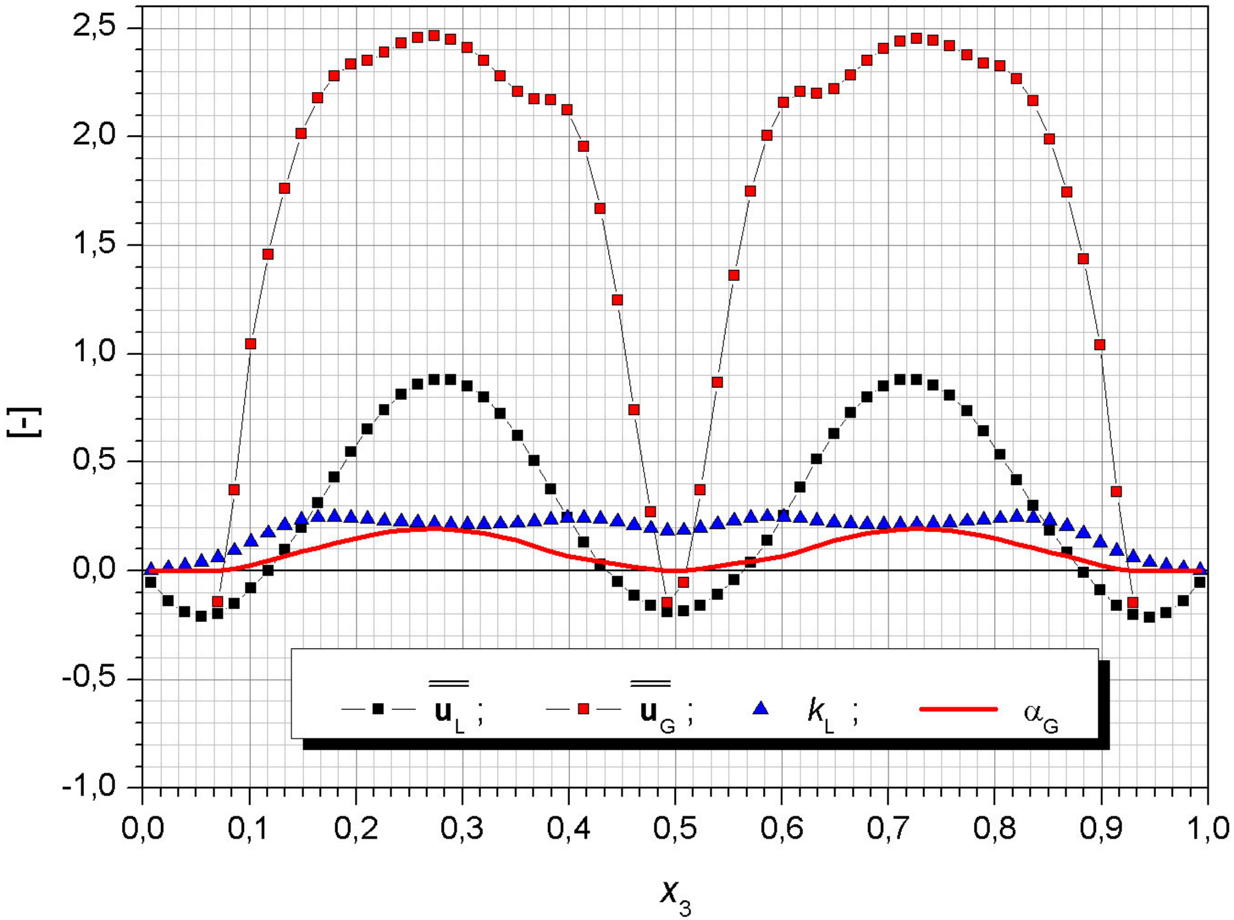
Wall-normal profiles of mean quantities

Plane averaging:

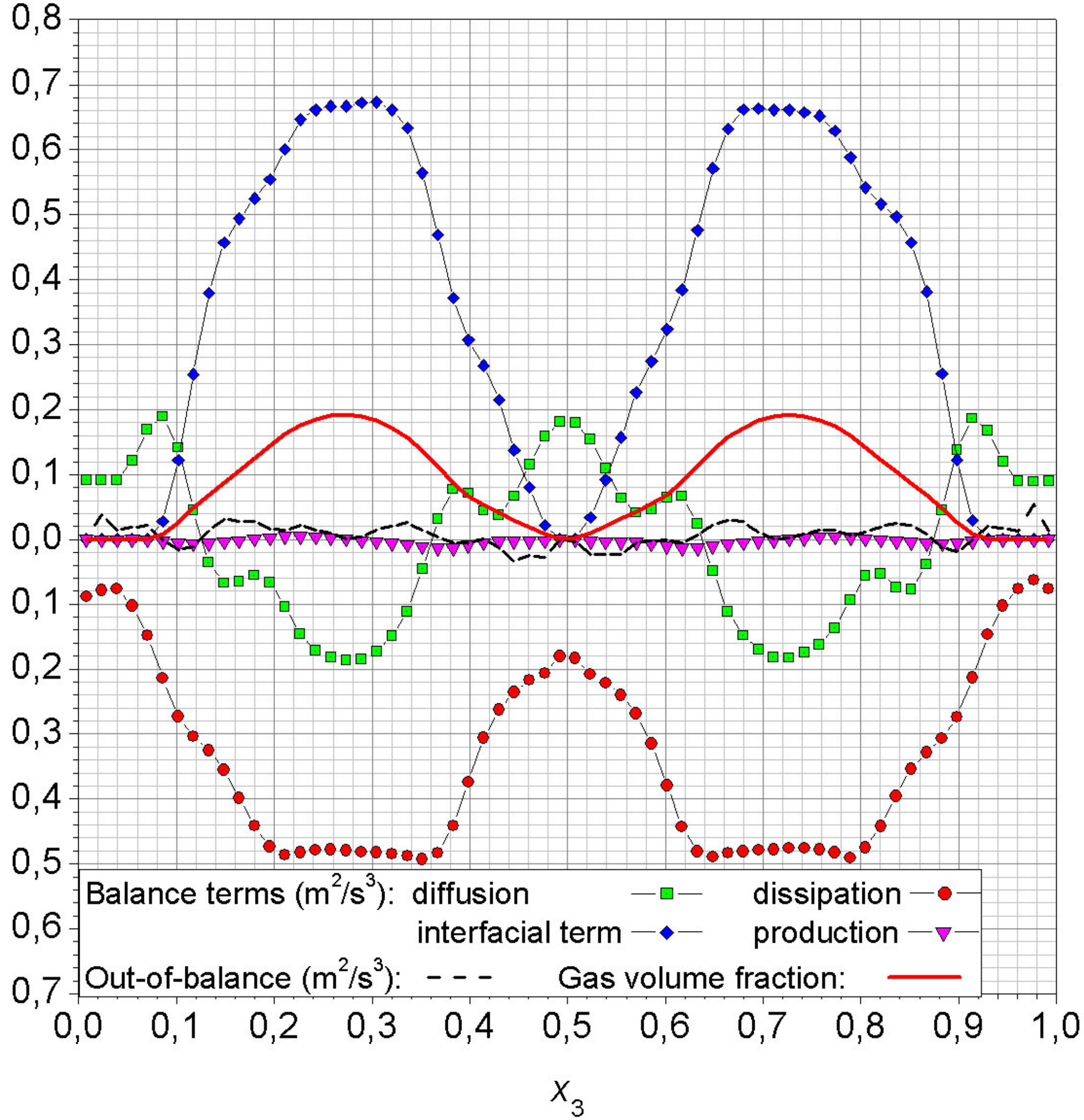
$$\overline{A_L}(x_3) = \frac{1}{N_1 N_2}\sum_{i=1}^{N_1}\sum_{j=1}^{N_2} f_{i,j,k}A_{i,j,k}$$

$$\overline{\overline{A_L}}(x_3) = \frac{\sum_{i=1}^{N_1}\sum_{j=1}^{N_2} f_{i,j,k}A_{i,j,k}}{\sum_{i=1}^{N_1}\sum_{j=1}^{N_2} f_{i,j,k}}$$





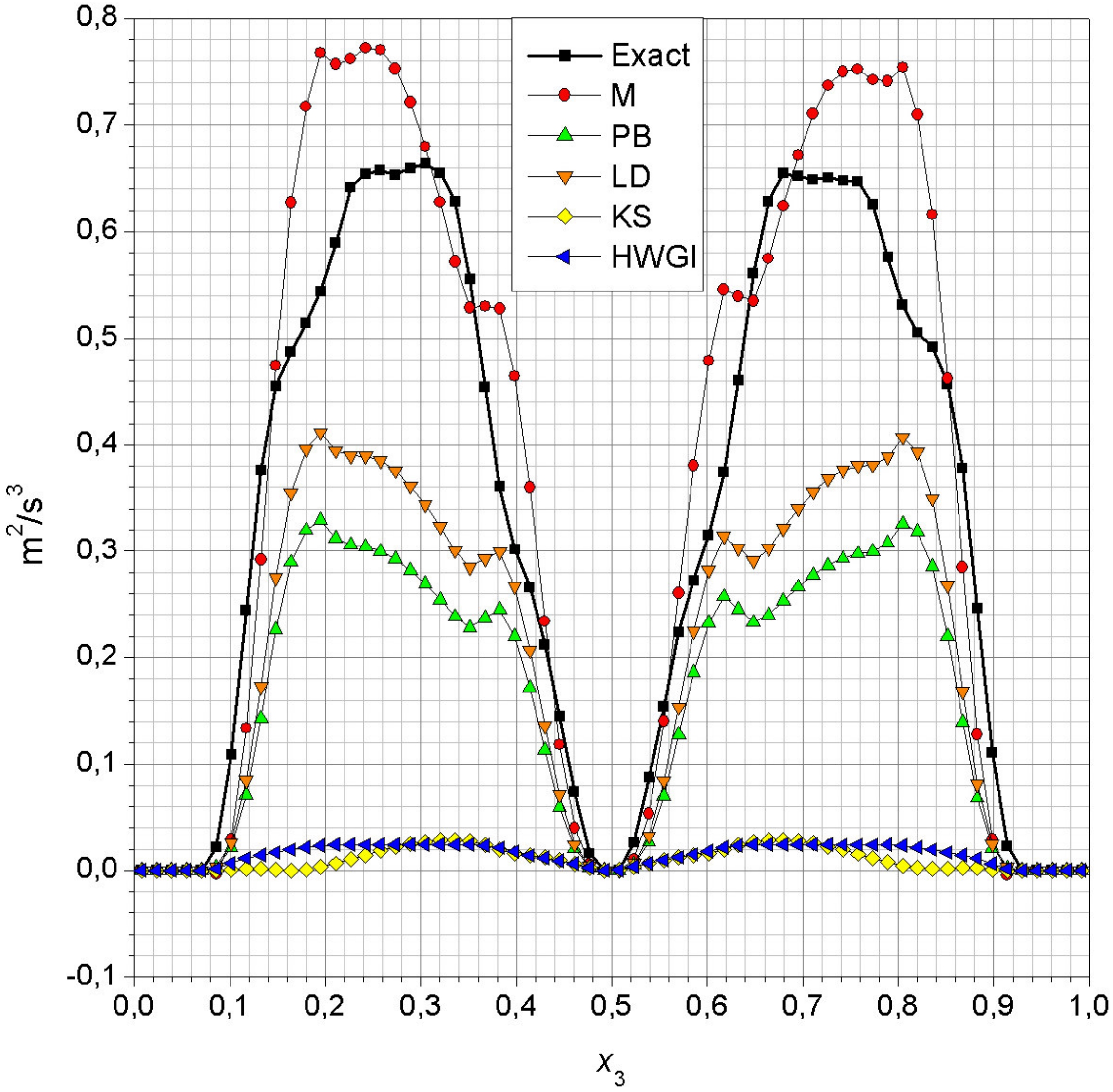
Budget of k_L-equation



Models for interfacial term

Reference	Work of drag force, W_D^*	Other contributions, W_{ND}^*
Kataoka & Serizawa (1997) Model 1, KS	$0.075 f_w \left[\frac{3}{4} \alpha_G \frac{C_D}{d_B^*} U_T^{*3} \right]$	$-\alpha_G \frac{k_L^{*3/2}}{d_B^*}$
Hill *et al.* (1995) Model 2, HWGI	$\frac{3}{4} \frac{\alpha_G C_D}{d_B^*} \lvert \overline{\overline{\mathbf{u}}}_R^* \rvert \left\{ \frac{\mu_L^* \overline{\overline{\mathbf{u}}}_R^* \cdot \nabla^* \alpha_G}{0.3 \rho_L^* \alpha_L \alpha_G} + 2k_L^* (C_t - 1) \right\}$	None
Lahey & Drew (2000) Model 3, LD	$\frac{1}{4} \alpha_L \left(1 + C_D^{4/3}\right) \alpha_G \frac{\lvert \overline{\overline{\mathbf{u}}}_R^* \rvert^3}{d_B^*}$	None
Morel (1997) Model 4, M	$\frac{3}{4} \alpha_G \frac{C_D}{d_B^*} \lvert \overline{\overline{\mathbf{u}}}_R^* \rvert^3$	$\frac{1 + 2\alpha_G}{2\alpha_L} \alpha_G \left\{ \frac{D_G \overline{\overline{\mathbf{u}}}_G^*}{Dt^*} - \frac{D_L \overline{\overline{\mathbf{u}}}_L^*}{Dt^*} \right\} \cdot \overline{\overline{\mathbf{u}}}_R^*$
Pfleger & Becker (2001) Model 5, PB	$1.44 \alpha_L \left[\frac{3}{4} \alpha_G \frac{C_D}{d_B^*} \lvert \overline{\overline{\mathbf{u}}}_R^* \rvert^3 \right]$	None

Performance of models for interfacial term



Conclusions

- Numerical simulation of bubble train flow
  - Square vertical mini-channel (2 mm × 2 mm)
  - Good agreement with experimental data from literature
  - Investigation on influence of length of flow unit cell
  - Strong influence of capillary number
- Liquid turbulence kinetic energy equation for bubbly flow
  - production mainly by interfacial terms
  - no local equilibrium between interfacial production and dissipation
    $\Rightarrow$ significant redistribution by diffusion
  - interfacial terms can well be modeled by work of drag forces