Karlsruher Institut für Technologie

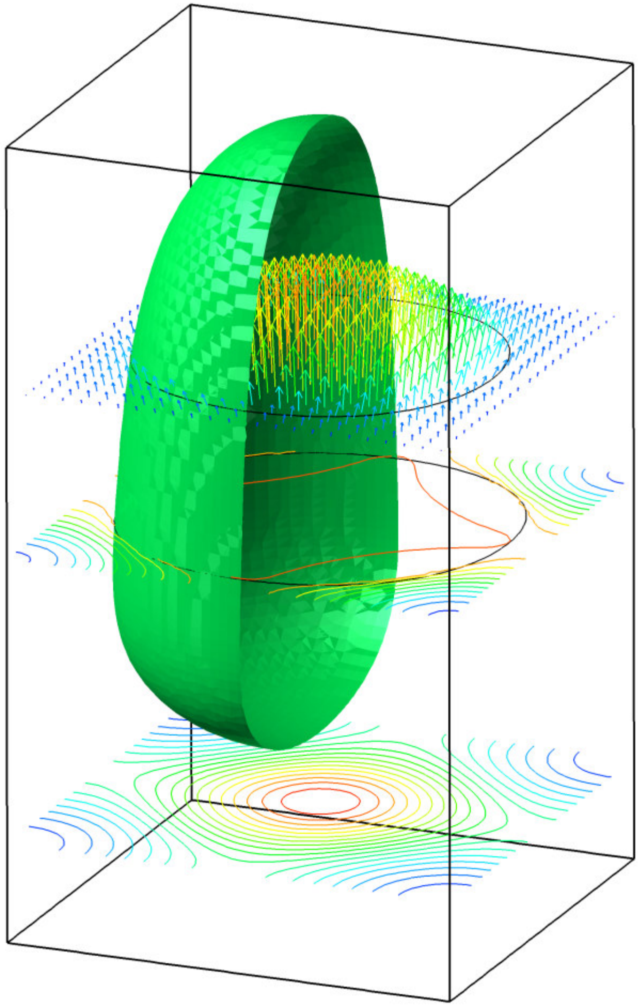
Mehrphasenströmungen und Transportvorgänge in der Mikroverfahrenstechnik

- *simulieren*
- *verstehen*
- *modellieren*

Dr.-Ing. Martin Wörner

Karlsruher Institut für Technologie
Institut für Katalyseforschung und –Technologie

Seminarvortrag am IMM, 9. Juli 2013

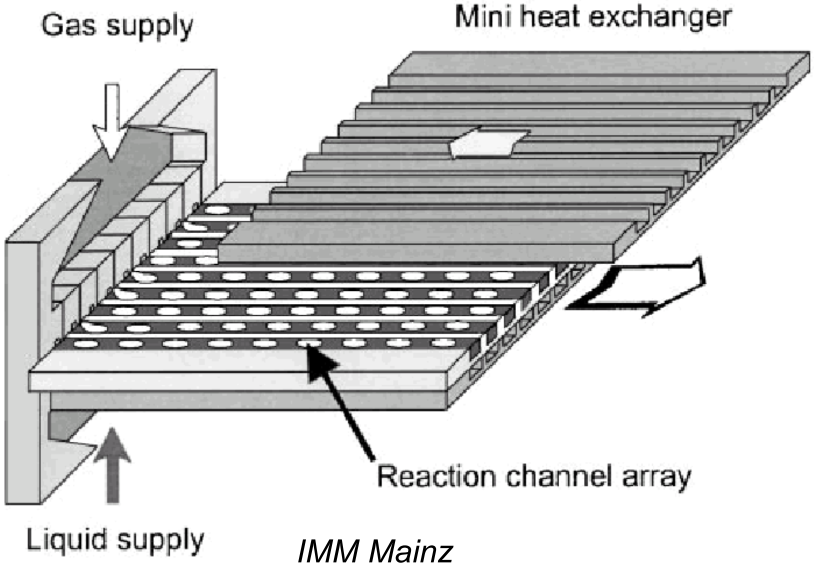


Taylor-Strömung mit Stofftransport in einem quadratischen Mini-Kanal

Outline

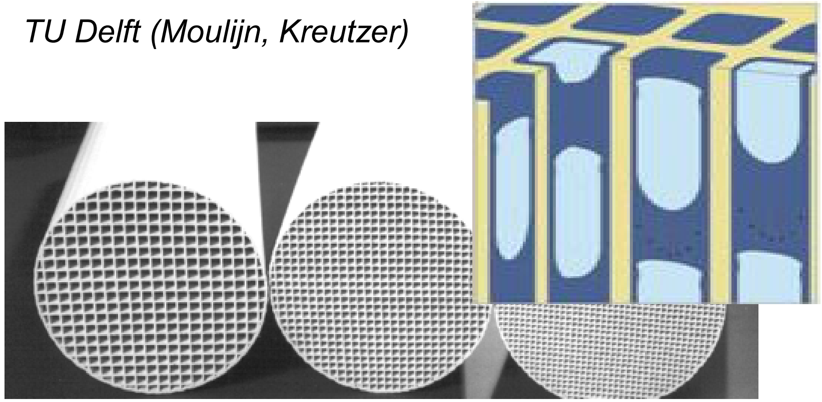
- Introduction
- Computational fluid dynamics in micro process engineering
  - Status and developments
- Taylor flow in square capillaries
  - Numerical method and computational setup
  - Insight by scale-resolving simulations
  - Development of engineering models
    - Pressure drop
    - Residence time distribution
- Short survey on further ongoing projects in the group
- Summary

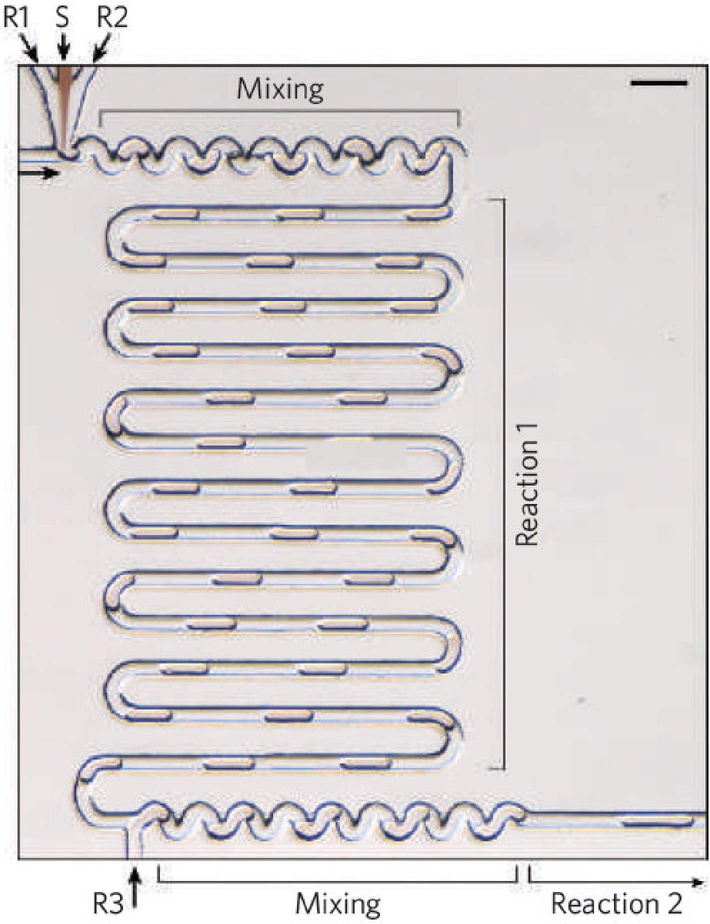
Multiphase micro reactors



IMM Mainz

TU Delft (Moulijn, Kreutzer)

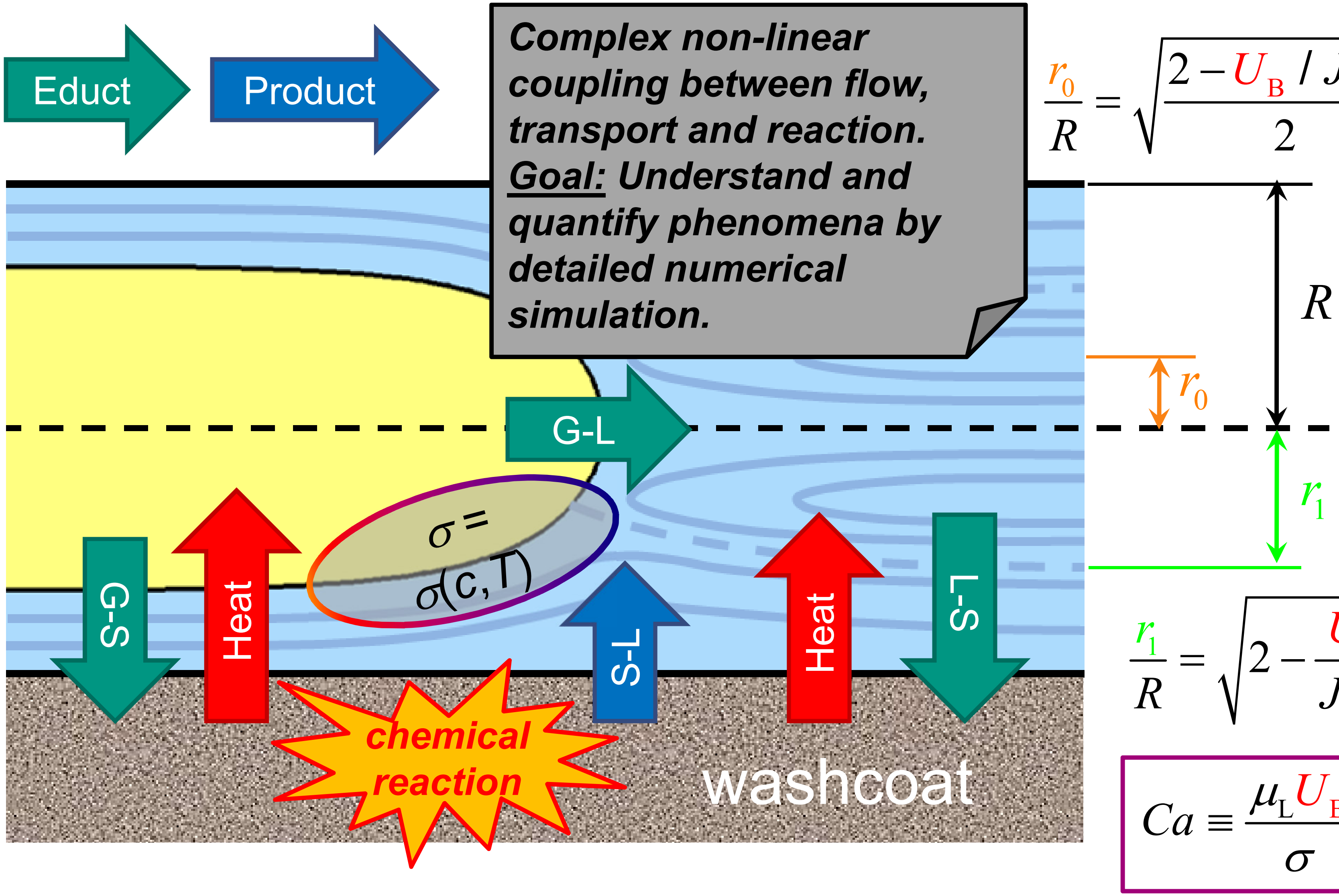




Univ. Chicago (Ismagilov et al.)

Flow, mass transfer, and reaction

Complex non-linear coupling between flow, transport and reaction.
<u>Goal:</u> Understand and quantify phenomena by detailed numerical simulation.



$$\frac{r_0}{R} = \sqrt{\frac{2 - U_B / J_{total}}{2}}$$

$$\frac{r_1}{R} = \sqrt{2 - \frac{U_B}{J_{total}}}$$

$$\boxed{Ca \equiv \frac{\mu_L U_B}{\sigma}}$$

Outline

- Introduction
- Computational fluid dynamics in micro process engineering
  - Status and developments
- Taylor flow in square capillaries
  - Numerical method and computational setup
  - Insight by scale-resolving simulations
  - Development of engineering models
    - Pressure drop
    - Residence time distribution
- Short survey on further ongoing projects in the group
- Summary

Single-field Navier-Stokes eqs.

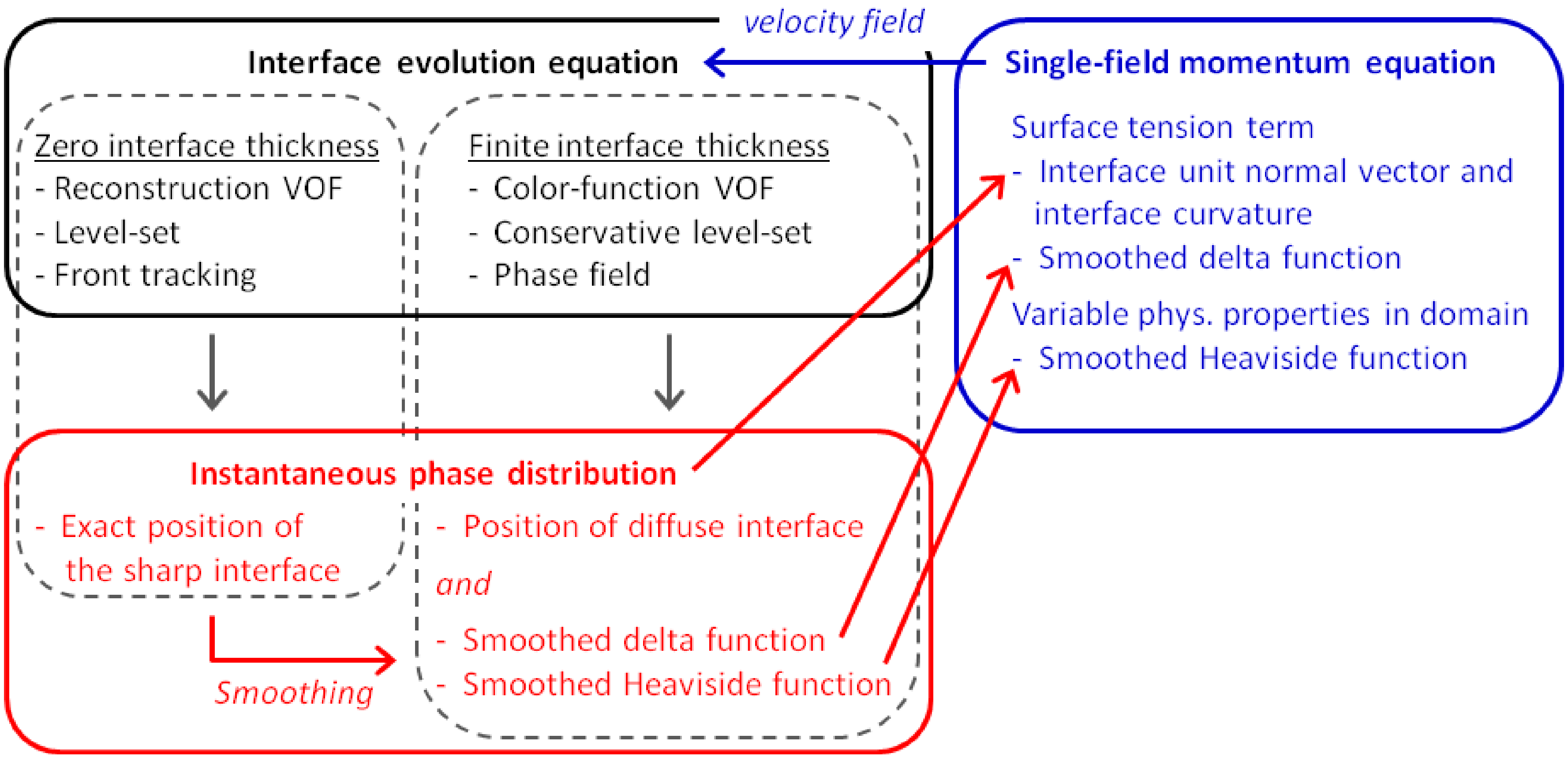
- Two incompressible Newtonian fluids with constant viscosities

$$\left.\begin{aligned} &\nabla\cdot\mathbf{v}=0 \\ &\frac{\partial\rho\mathbf{v}}{\partial t}+\nabla\cdot\left(\rho\mathbf{v}\otimes\mathbf{v}\right)=-\nabla p+\nabla\cdot\mu\left(\nabla\mathbf{v}+(\nabla\mathbf{v})^{\mathrm{T}}\right) \\ &\qquad +\rho\mathbf{g}+\left(\sigma\kappa\hat{\mathbf{n}}_\Gamma+\nabla_\Gamma\sigma\right)\delta_\Gamma \end{aligned}\right\} \quad \mathbf{x}\in\Omega\neq\Omega(t)$$

Eqs. are valid in entire domain

- Density $\rho(\mathbf{x},t)$ and viscosity $\mu(\mathbf{x},t)$ are piecewise constant in each phase but are discontinuous at the interface
- Surface tension term
  - κ = interface curvature
  - δ_Γ = Dirac delta function with support on the interface
- *A method for describing the phase distribution is required!*

Coupling between interface evolution and momentum eq.



velocity field

Interface evolution equation

Zero interface thickness
- Reconstruction VOF
- Level-set
- Front tracking

Finite interface thickness
- Color-function VOF
- Conservative level-set
- Phase field

Single-field momentum equation

Surface tension term
- Interface unit normal vector and interface curvature
- Smoothed delta function

Variable phys. properties in domain
- Smoothed Heaviside function

Instantaneous phase distribution

- Exact position of the sharp interface

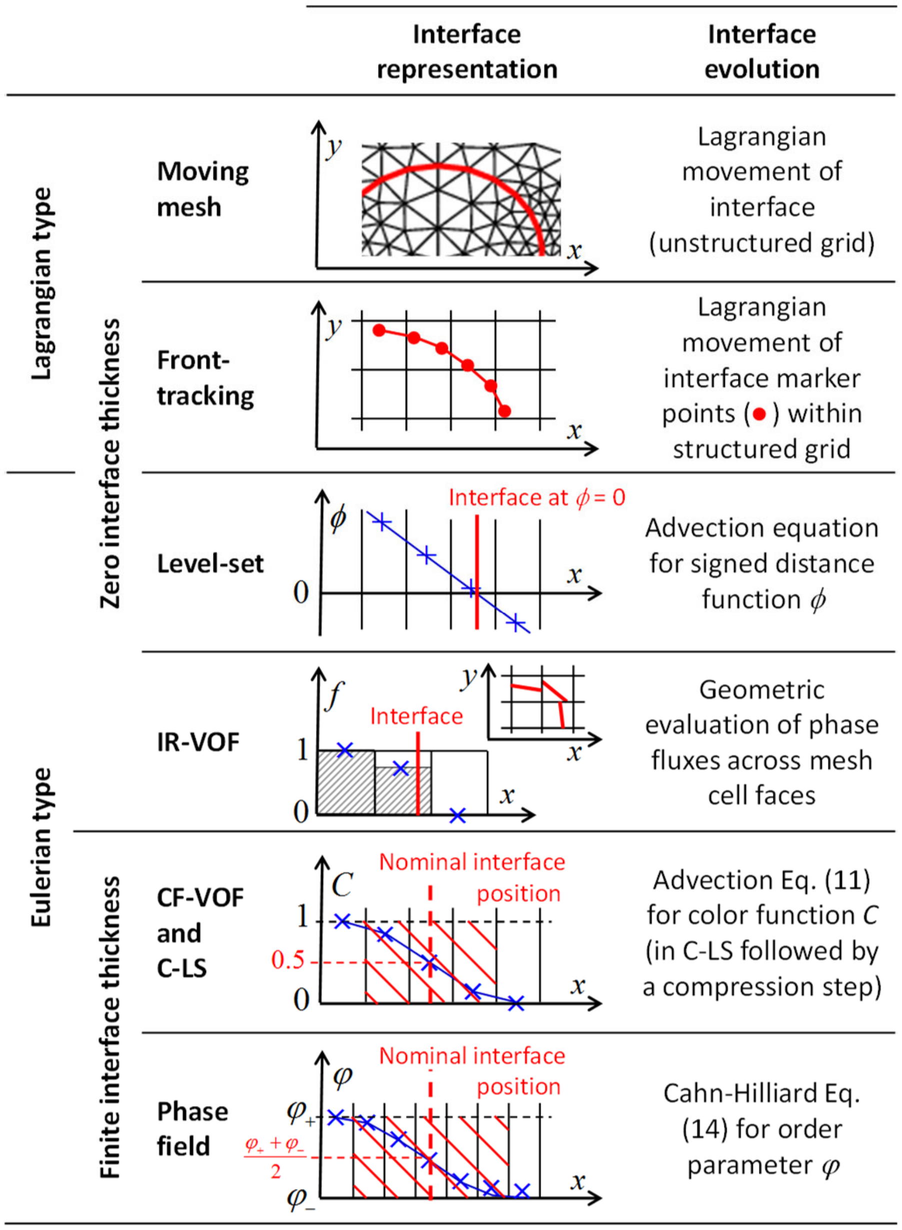
Smoothing

- Position of diffuse interface

and

- Smoothed delta function
- Smoothed Heaviside function

W., Microfluid Nanofluid **12** (2012) 841-886



			Interface representation	Interface evolution
Lagrangian type	Zero interface thickness	Moving mesh		Lagrangian movement of interface (unstructured grid)
		Front-tracking		Lagrangian movement of interface marker points (●) within structured grid
Eulerian type		Level-set		Advection equation for signed distance function ϕ
		IR-VOF		Geometric evaluation of phase fluxes across mesh cell faces
	Finite interface thickness	CF-VOF and C-LS		Advection Eq. (11) for color function C (in C-LS followed by a compression step)
		Phase field		Cahn-Hilliard Eq. (14) for order parameter φ

- **Moving mesh method**
  - \+ Interface does not cut cells but separates phases
  - – Adaptive grid required; difficulty in handling break-up and coalescence
- **Front-tracking method**
  - \+ Does not impose artificial coalescence as VOF and LS method often do
  - – Complexity in handling break-up/coalescence
- **Level-set method**
  - \+ Avoids interface reconstruction;
    flexibility in handling topological changes
  - – Special measures necessary to reduce mass conservation errors
- **Volume-of-fluid method with interface reconstruction**
  - \+ Very good mass conservation
  - – Complex interface reconstruction/advection algorithms in 3D
- **Color-function VOF and conservative level-set meth.**
  - \+ Methods are rather easy to implement
  - – Special measures necessary to keep the interface thickness constant and uniform
- **Phase-field method**
  - \+ Allows for effective control of interface thickness; can handle moving contact lines
  - – For accurate results the diffuse interface region must be adequately resolved

W., Microfluid Nanofluid **12** (2012) 841-886

SPP 1506 Benchmark Taylor Flow

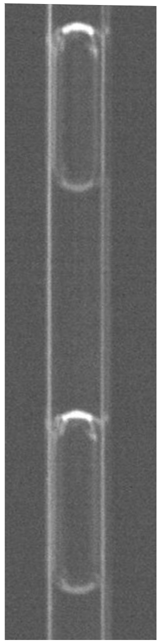
KIT
Karlsruher Institut für Technologie

DFG Deutsche Forschungsgemeinschaft

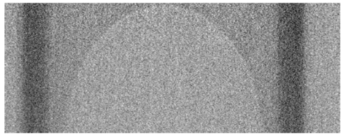
Transport processes at fluidic interfaces
DFG SPP 1506

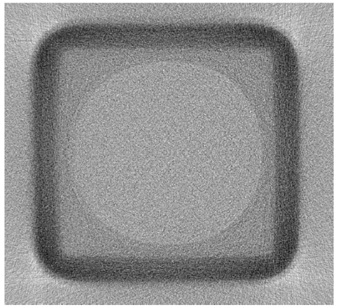
- SPP 1506 “Transport Processes at fluidic interfaces”
  - Guiding measure Taylor flow
  - Goal: establish benchmarks for detailed quantitative validation of CFD method and codes
- Measurements by experimental groups
  - d_h= 2 mm capillary with circular / square cross section
  - water-glyzerine solution / air; co-current upward flow
  - Single Taylor bubble: Boden/Hampel HZDR
  - Taylor flow: Meyer/Schlüter TUHH
- **TBSC** = **T**aylor **B**ubble **S**quare **C**hannel (3D)
  - contour of bubble shape (lateral and diagonal plane)
- **TFSC** = Taylor **F**low **S**quare **C**hannel (3D)
  - velocity profiles from µPIV in liquid slug and liquid film
- **TBCC** = Taylor **B**ubble **C**ircular **C**hannel (2½D)
  - contour of bubble shape


HZDR


TUHH

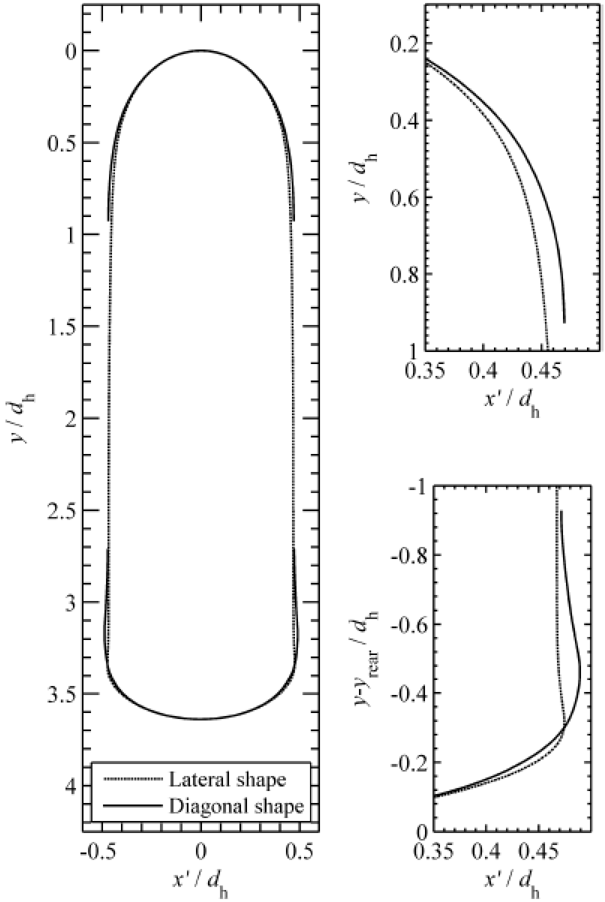
Case Taylor Bubble Square Channel



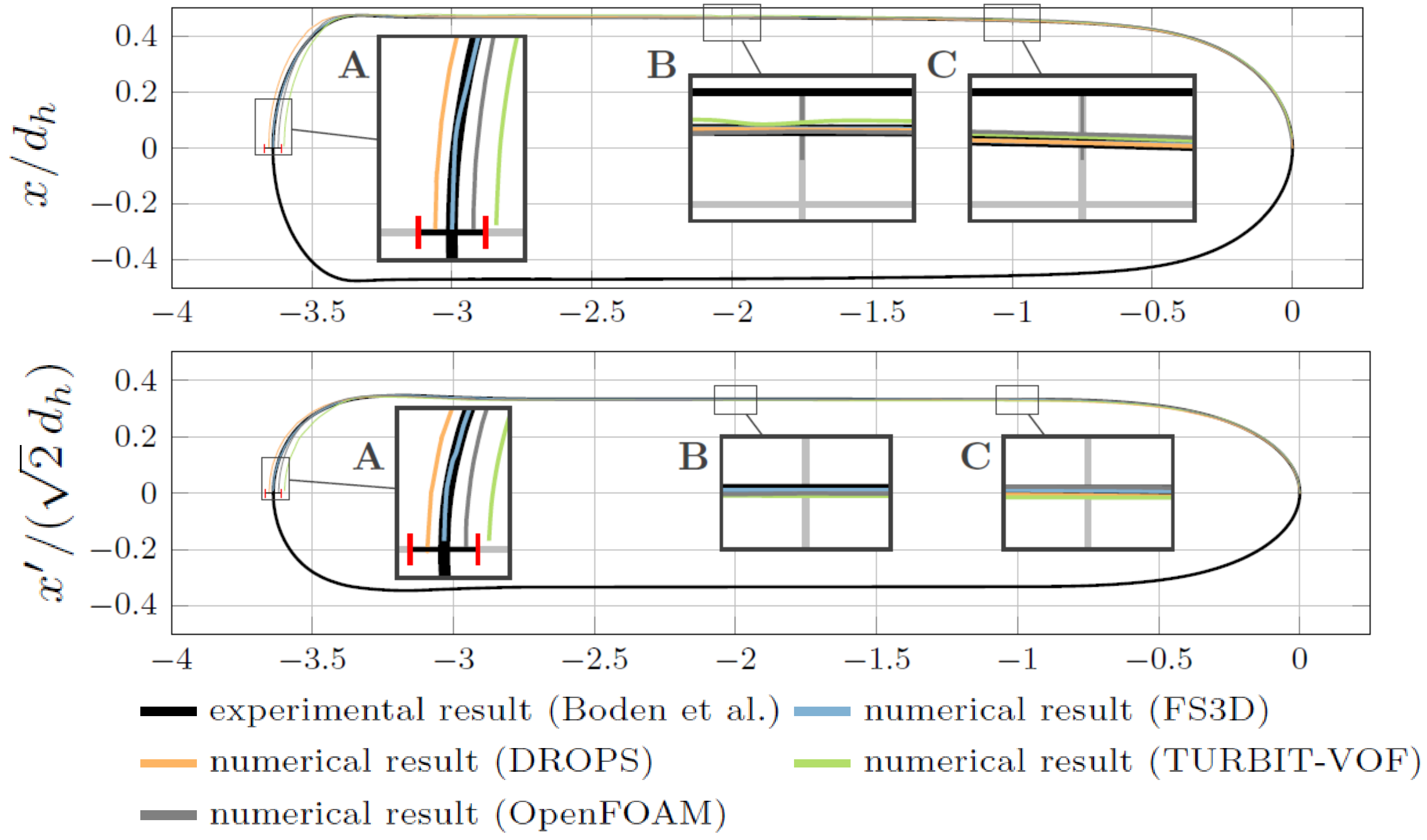


S. Boden,
U. Hampel

Bubble is not axi-symmetric!



Comparison of numerical methods[*,#]



[*] Marschall, Boden, Lehrenfeld, Falconi, Hampel, Reusken, W., Bothe; Computers & Fluids (accepted)

[#] For 2D test case see Aland et al., Int. J. Num. Meth. Fluids (accepted, available online)

Interface resolving simulations: status and ongoing developments

- Hydrodynamics of two-phase flow including bubble and drop formation ✓
- *Coalescence phenomena* 👓
- *Mass transfer (realistic Schmidt numbers)* 👓
- *Interfacial transport of soluble and insoluble surfactants* 👓
- *Coupling of two-phase flow and transport with chemical kinetics* 👓

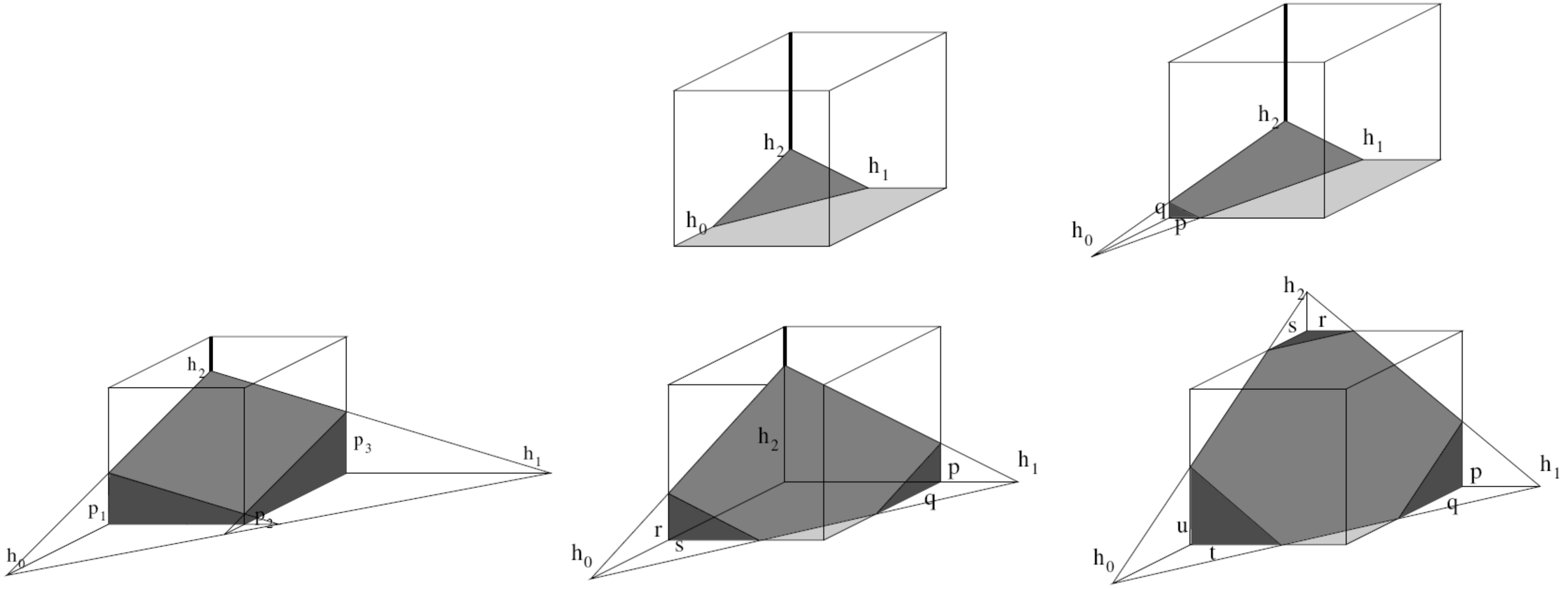
New SPP 1740 Reactive Bubbly Flows (Prof. M. Schlüter, TUHH)

Outline

- Introduction
- Computational fluid dynamics in micro process engineering
  - Status and developments
- Taylor flow in square capillaries
  - Numerical method and computational setup
  - Insight by scale-resolving simulations
  - Development of engineering models
    - Pressure drop
    - Residence time distribution
- Short survey on further ongoing projects in the group
- Summary

Simulation method*

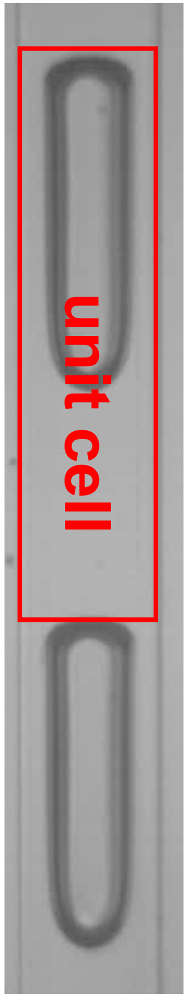
- In-house computer code TURBIT-VOF
  for details see Öztaskin et al. Phys. Fluids **21** (2009) 042108
- Volume-of-fluid method with piecewise linear interface reconstruction

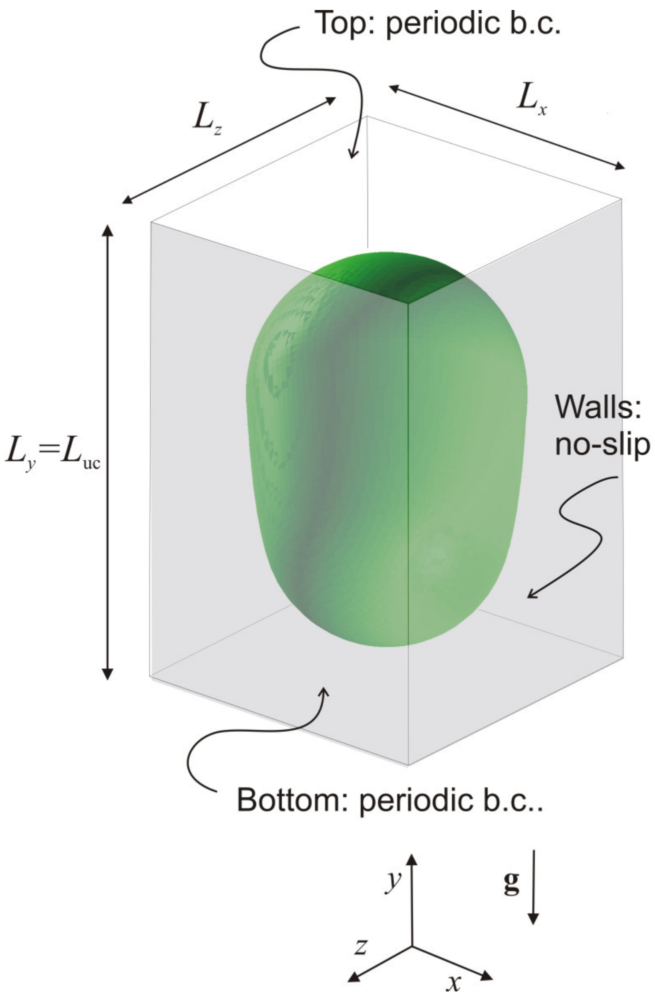


- Finite volume discretization an a staggered 3D Cartesian grid
- Projection method for pressure-velocity coupling
- Explicit 3rd order Runge-Kutta time integration scheme

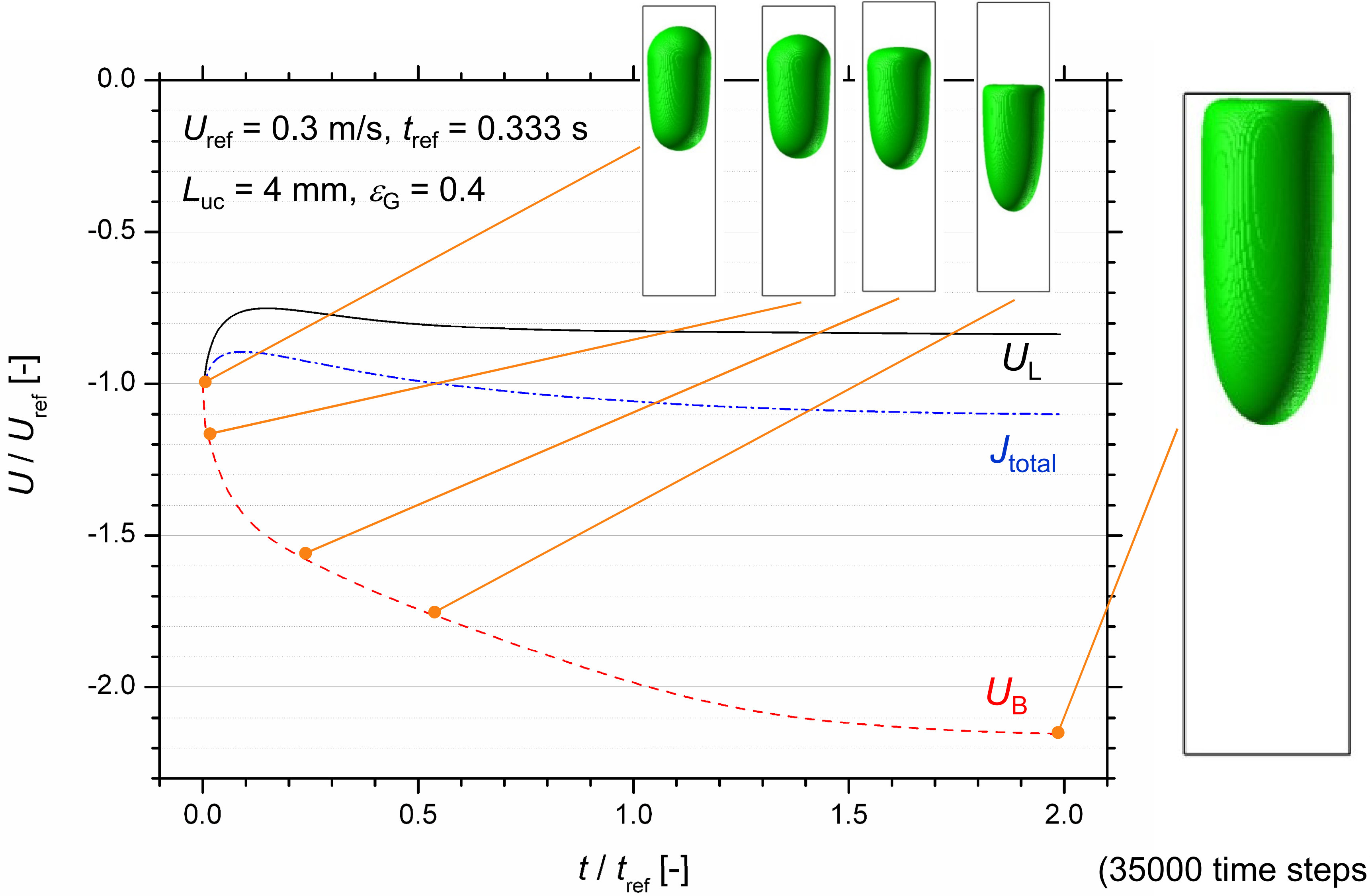
Computational set-up for Taylor flow

- Set-up
  - Co-current downward flow of squalane ($C_{30}H_{62}$) and nitrogen
  - Square channel (hydraulic diameter D_h = 0.5, 1, 2, 4 mm)
  - Consideration of **one unit cell**
  - Periodic boundary conditions in vertical (axial) direction
- Prescribed parameters
  - Gas content: ε_G = 0.2 or 0.4
  - Unit cell length: L_y / D_h = 4 or 6 (grid up to 80 × 480 × 80 cells)
  - Pressure drop across the unit cell $Eu_{ref} = \Delta p_{uc} / (\rho_L U_{ref}^2)$





Evolution in time



(35000 time steps)

Steady bubble shape for D_h = 1 mm

$1\,\mathrm{mm} \times 1\,\mathrm{mm}$

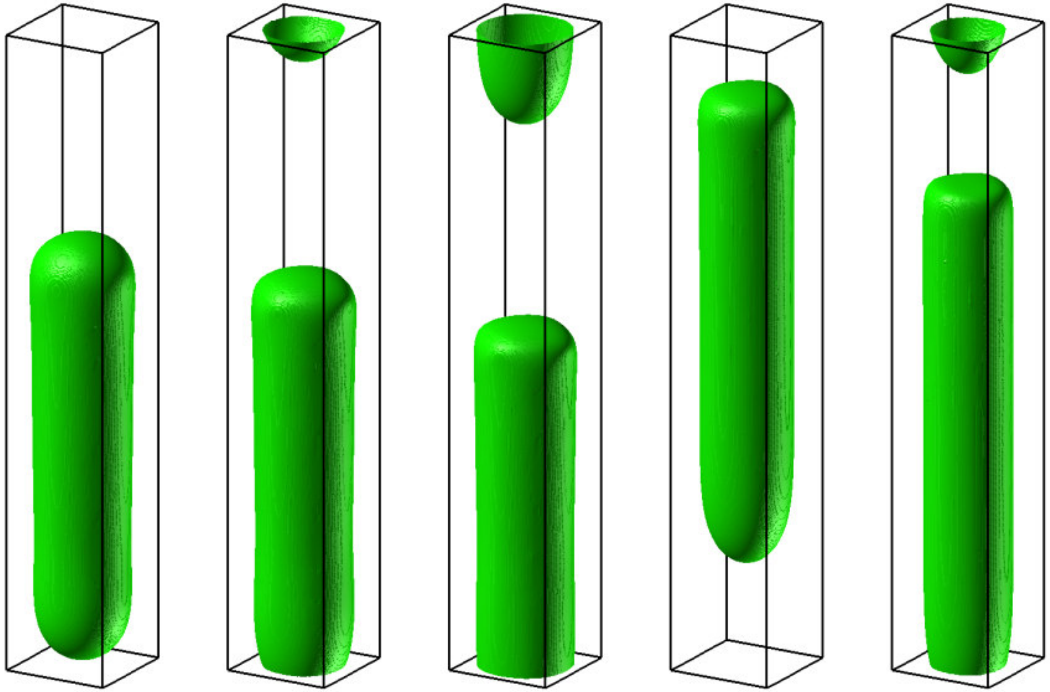
$L_{\mathrm{uc}} = 6\,\mathrm{mm}$

$\varepsilon_{\mathrm{G}} = 0.4$

$$Ca_{\mathrm{B}} = \frac{\mu_{\mathrm{L}} U_{\mathrm{B}}}{\sigma}$$

$$Re_{\mathrm{B}} = \frac{\rho_{\mathrm{L}} D_{\mathrm{h}} U_{\mathrm{B}}}{\mu_{\mathrm{L}}}$$

$$La = \frac{\sigma \rho_{\mathrm{L}} D_{\mathrm{h}}}{\mu_{\mathrm{L}}^2} = 27.27$$



Ca_{B} =	0.045	0.12	0.17	0.26	0.49
Re_{B} =	1.22	3.19	4.64	7.16	13.4

Increase of Ca_{B} and $Re_{\mathrm{B}} = La\, Ca_{\mathrm{B}}$

Increase of δ_{F}, L_{B}, κ_{front} (curvature of front meniscus)
Decrease of D_{B}, L_{slug}, κ_{rear} (curvature of rear meniscus)

Channel size effects in Taylor flow

- Size 0.5 × 0.5 mm

  $D_\mathrm{h} = 0.5$ mm

  $Ca_\mathrm{B} = 0.202$

  $Re_\mathrm{B} = 2.75$

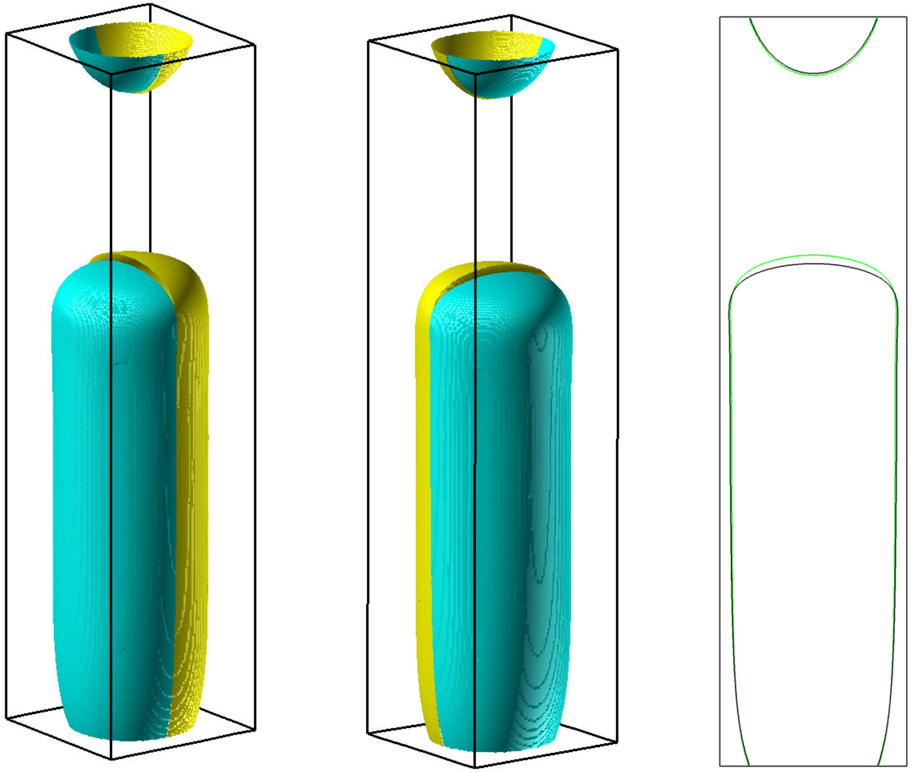
  $E\ddot{o} = 0.067$
- Size 2 × 2 mm

  $D_\mathrm{h} = 2.0$ mm

  $Ca_\mathrm{B} = 0.213$

  $Re_\mathrm{B} = 11.6$ (inertia)

  $E\ddot{o} = 1.068$ (buoyancy)

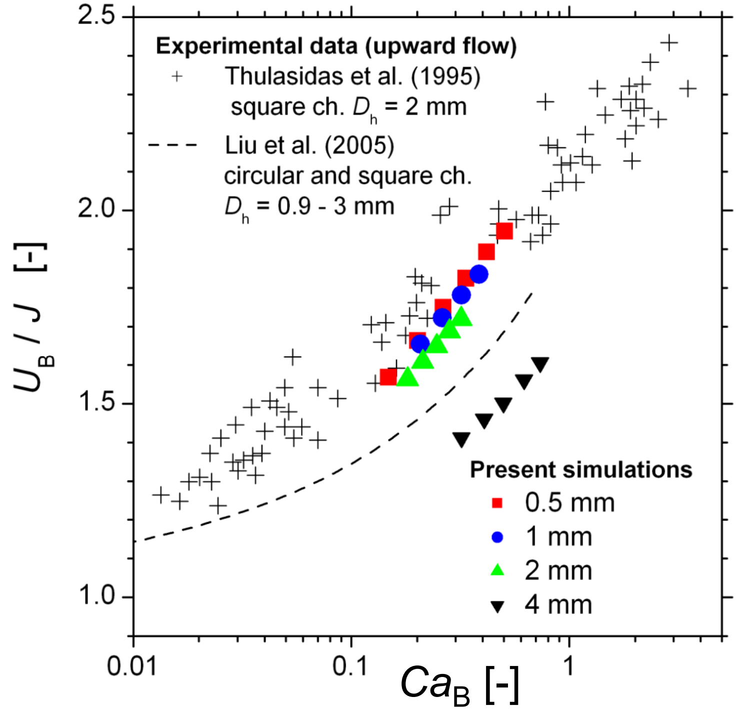


- Combined influence of Re_B and $E\ddot{o}$ for fixed value of Ca_B
  - Very small influence on $\delta_\mathrm{F}/D_\mathrm{h}$ (film thickness) and $\kappa_\mathrm{front}\,D_\mathrm{h}$
  - Notable influence on $\kappa_\mathrm{rear}\,D_\mathrm{h}$ (inertial effect, known in literature)

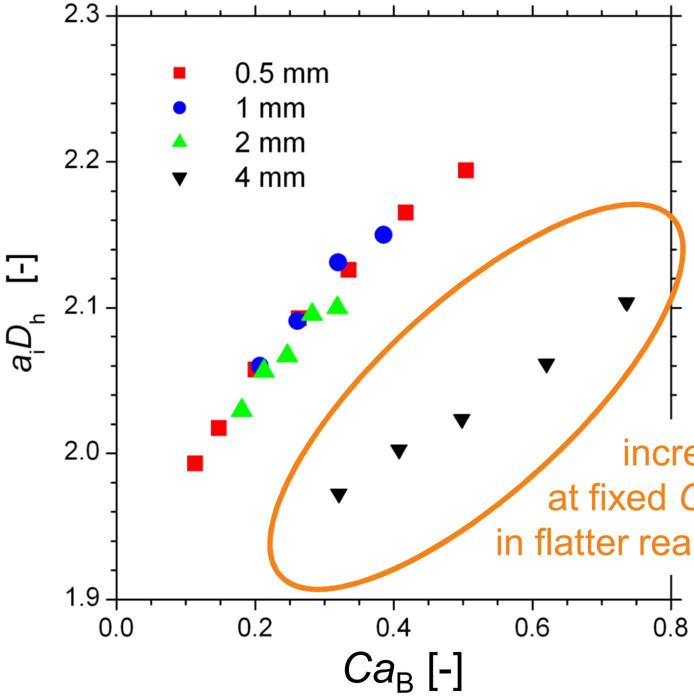
W., J. Chem. Eng. Japan **46** (2013) 335

Influence of channel size

Non-dimensional bubble velocity



Non-dim. specific interfacial area

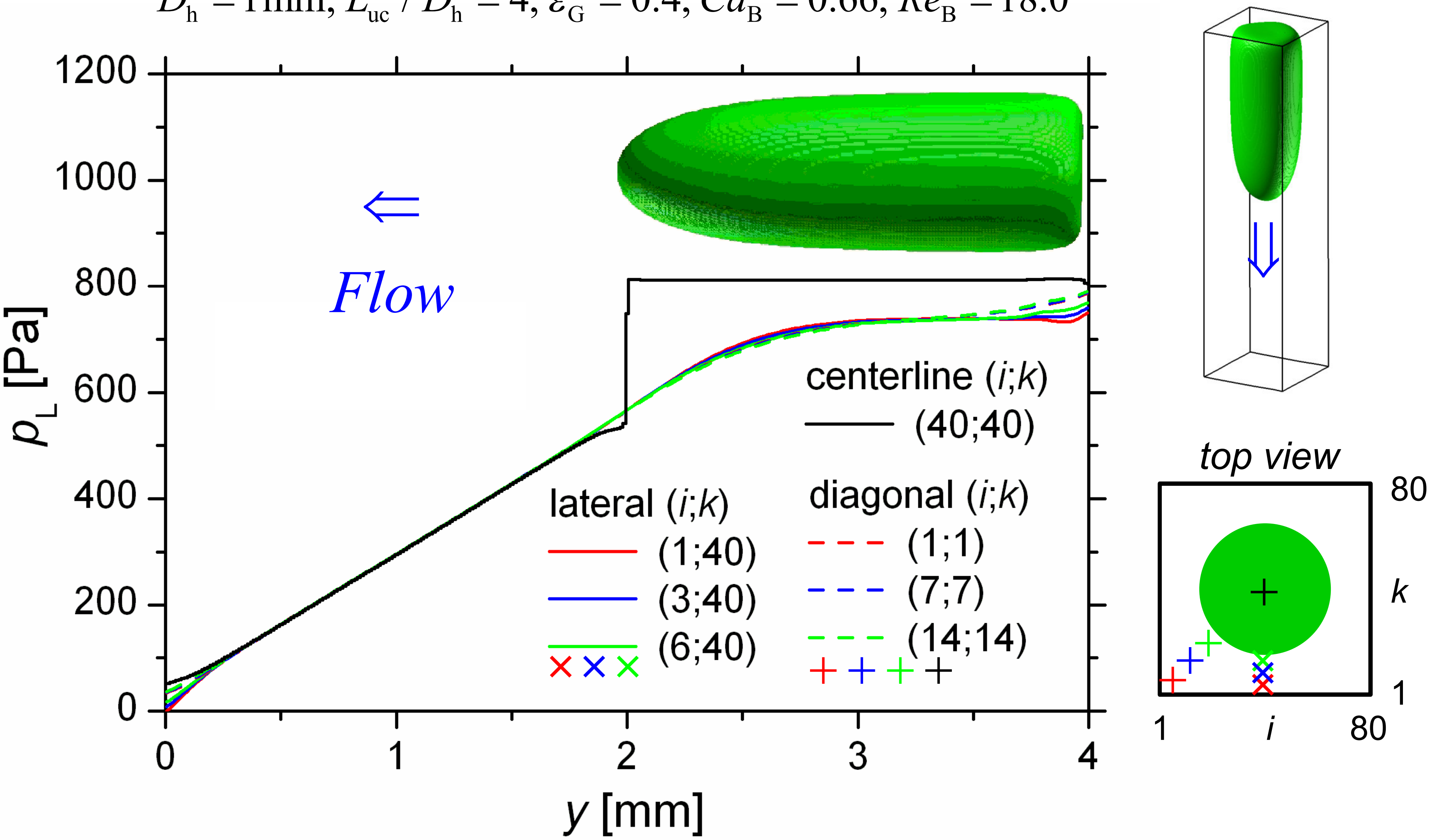


increase of *Re* at fixed Ca_B results in flatter rear meniscus

- For $D_h \leq 2$ mm the influence of inertia (Re_B) and buoyancy ($Eö$) is very small → ***scaling with*** $\boldsymbol{Ca_B}$
- For $D_h > 2$ mm the influence of inertia and buoyancy become important

Axial profiles of liquid pressure

$D_\mathrm{h} = 1\,\mathrm{mm},\ L_\mathrm{uc} / D_\mathrm{h} = 4,\ \varepsilon_\mathrm{G} = 0.4,\ Ca_\mathrm{B} = 0.66,\ Re_\mathrm{B} = 18.0$



Outline

- Introduction
- Computational fluid dynamics in micro process engineering
  - Status and developments
- Taylor flow in square capillaries
  - Numerical method and computational setup
  - Insight by scale-resolving simulations
  - Development of engineering models
    - Pressure drop
    - Residence time distribution
- Short survey on further ongoing projects in the group
- Summary

Pressure drop models in literature

*Kreutzer et al.** *Warnier et al.#*

- Hydrodynamic pressure drop in a unit cell

$$-\left(\frac{\mathrm{d}P}{\mathrm{d}z}\right)_{\mathrm{uc}} = -\left(\frac{\mathrm{d}P}{\mathrm{d}z}\right)_{\mathrm{slug}}\left(\frac{L_{\mathrm{slug}}}{L_{\mathrm{bubble}}+L_{\mathrm{slug}}}\right) \qquad -\left(\frac{\mathrm{d}P}{\mathrm{d}z}\right)_{\mathrm{uc}} = -\left(\frac{\mathrm{d}P}{\mathrm{d}z}\right)_{\mathrm{slug}}\left(\frac{L_{\mathrm{slug}}+D_B/3}{L_{\mathrm{bubble}}+L_{\mathrm{slug}}}\right)$$

- Frictional pressure drop in the liquid slug

$$-\left(\frac{\mathrm{d}P}{\mathrm{d}z}\right)_{\mathrm{slug}} = 32\frac{\mu_{\mathrm{L}}J_{\mathrm{total}}}{D_{\mathrm{h}}^2}\left(1+a\frac{D_h}{L_{\mathrm{slug}}}La^{0.33}\right) \qquad -\left(\frac{\mathrm{d}P}{\mathrm{d}z}\right)_{\mathrm{slug}} = 32\frac{\mu_{\mathrm{L}}J_{\mathrm{total}}}{D_{\mathrm{h}}^2}\left(1+a\frac{D_h}{L_{\mathrm{slug}}+D_B/3}La^{0.33}\right)$$

$$J_{\mathrm{total}} = J_{\mathrm{G}} + J_{\mathrm{L}}, \quad La = \sigma\rho_{\mathrm{L}}D_{\mathrm{h}}/\mu_{\mathrm{L}}^2$$

Models do not involve Ca_B or Re_B (only the ratio of both, La)

- Fitting coefficient

$a = 0.07$ numerical

$a = 0.17$ experimental

$a = 0.1$ experimental

*Kreutzer et al. AIChE J. **51** (2005) 2428

#Warnier et al. Microfluid Nanofluid **8** (2010) 33

Pressure drop model Boran & W.

- Goal: development of a “mechanistic” model for the hydrodynamic pressure drop along one unit cell
- The model shall involve only “a priori” known quantities
  - Physical properties ρ_L, μ_L, σ, g
  - Channel hydraulic diameter D_h
  - Superficial velocities $J_\mathrm{L}, J_\mathrm{G} \quad \rightarrow \quad J_\mathrm{total} = J_\mathrm{G} + J_\mathrm{L}$
  - The following non-dimensional numbers can be defined

$$\beta = \frac{J_\mathrm{G}}{J_\mathrm{total}}, \quad Ca_\mathrm{J} = \frac{\mu_L J_\mathrm{total}}{\sigma}, \quad La = \frac{\sigma \rho D_\mathrm{h}}{\mu_\mathrm{L}^2}$$

- The pressure drop along a unit cell consists of two parts
  - Pressure drop in the liquid slug
  - Pressure drop in the liquid film along the bubble

$$\boxed{\frac{\Delta P_\mathrm{uc}}{L_\mathrm{uc}} = \frac{\Delta P_\mathrm{slug}}{L_\mathrm{uc}} + \frac{\Delta P_\mathrm{film}}{L_\mathrm{uc}}}$$

Pressure drop in the liquid slug

- Analogous to Kreutzer et al.:

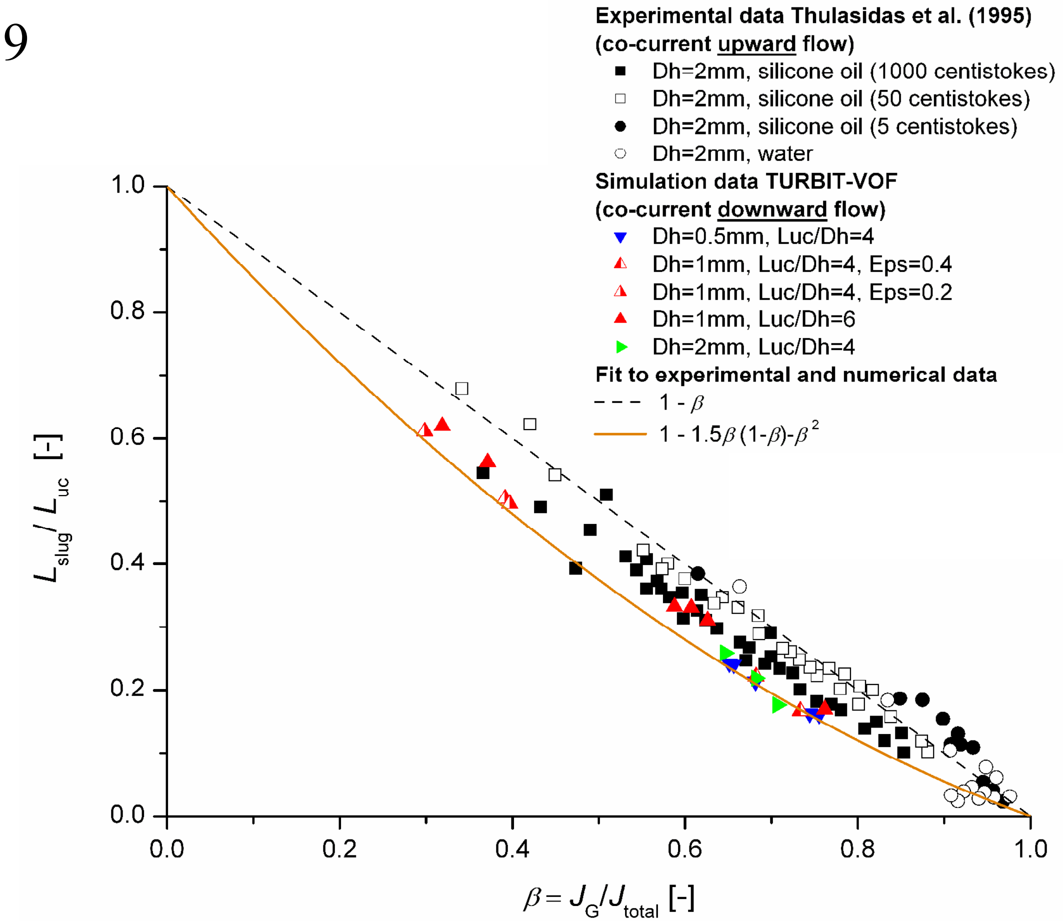
$$\frac{\Delta P_{\mathrm{slug}}}{L_{\mathrm{uc}}} = \left(\frac{\mathrm{d}P}{\mathrm{d}y}\right)_{\mathrm{slug}} \frac{L_{\mathrm{slug}}}{L_{\mathrm{uc}}} = \frac{C_{\mathrm{f}}}{2}\frac{\mu_{\mathrm{L}} J_{\mathrm{total}}}{D_{\mathrm{h}}^{2}}\frac{L_{\mathrm{slug}}}{L_{\mathrm{uc}}}$$

  - Round channel: $C_{\mathrm{f}} = 64$
  - Square channel: $C_{\mathrm{f}} = 56.9$
- The ratio $L_{\mathrm{slug}}/L_{\mathrm{uc}}$ is modeled by fitting of experimental and numerical data

$$\frac{L_{\mathrm{slug}}}{L_{\mathrm{uc}}} = 1 - C_{\mathrm{slug}}\beta(1-\beta) - \beta^{2}$$

$$C_{\mathrm{slug}} = 1 \quad \rightarrow \quad \frac{L_{\mathrm{slug}}}{L_{\mathrm{uc}}} = 1 - \beta$$

$$\text{Here:} \quad C_{\mathrm{slug}} = 1.5$$



Pressure drop along liquid film

- Young-Laplace equation at the front and rear meniscus

$$p_{\mathrm{B,front}} \approx p_{\mathrm{L,front}} + \sigma\kappa_{\mathrm{front}}, \qquad p_{\mathrm{B,rear}} \approx p_{\mathrm{L,rear}} + \sigma\kappa_{\mathrm{rear}}$$

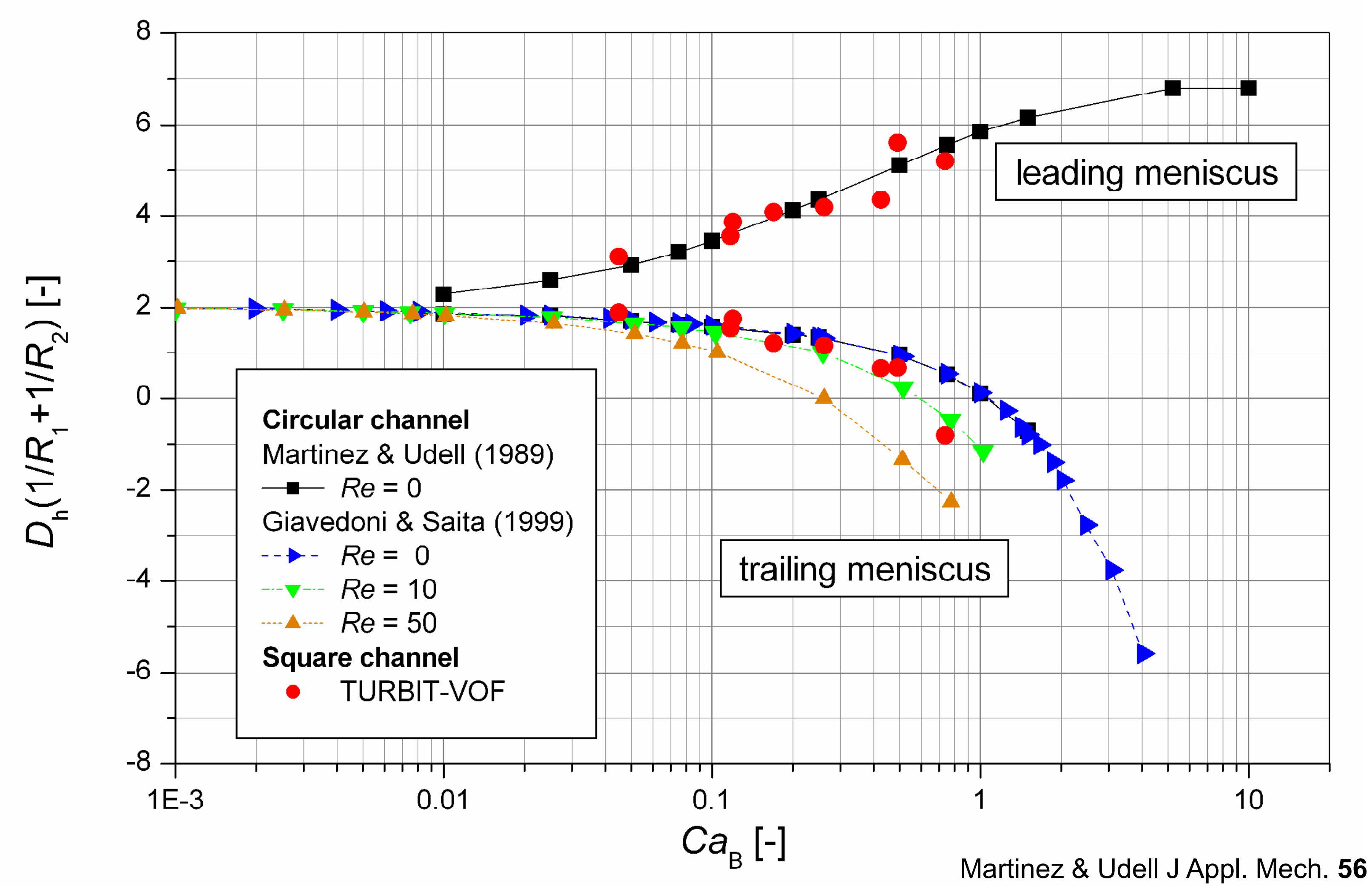
- The pressure in the bubble is about constant so that

$$\Delta P_{\mathrm{film}} = p_{\mathrm{L,rear}} - p_{\mathrm{L,front}} = \sigma(\kappa_{\mathrm{rear}} - \kappa_{\mathrm{front}})$$

$$\boxed{\frac{\Delta P_{\mathrm{film}}}{L_{\mathrm{uc}}} = (\kappa_{\mathrm{rear}} - \kappa_{\mathrm{front}})\frac{\sigma}{L_{\mathrm{uc}}} = (D_{\mathrm{h}}\kappa_{\mathrm{rear}} - D_{\mathrm{h}}\kappa_{\mathrm{front}})\frac{\sigma}{D_{\mathrm{h}}L_{\mathrm{uc}}}}$$

→ we need models for the non-dimensional bubble front and rear curvatures $D_{\mathrm{h}}\kappa_{\mathrm{rear}}$ and $D_{\mathrm{h}}\kappa_{\mathrm{front}}$

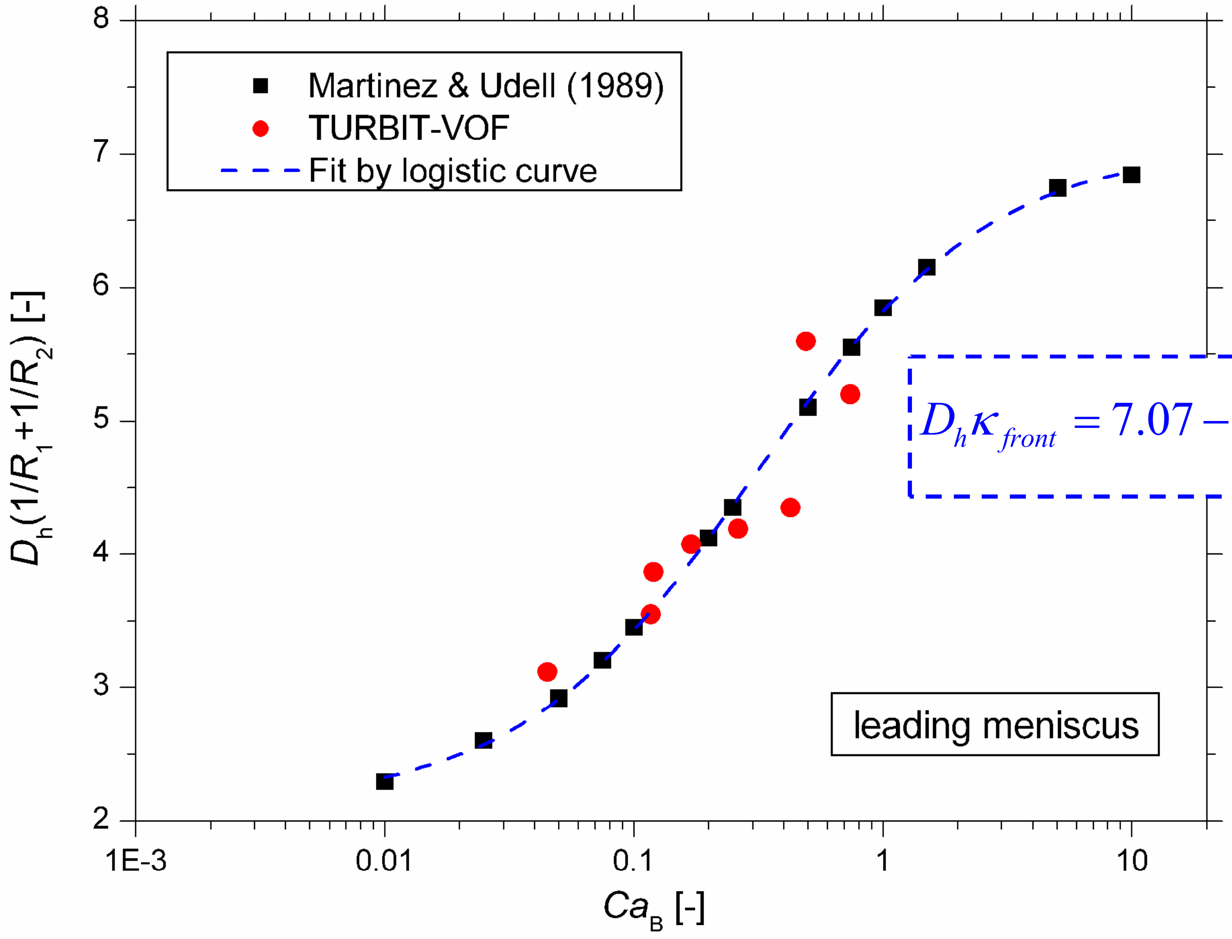
Data for front and rear curvature



Martinez & Udell J Appl. Mech. **56** (1989) 211
Giavedoni & Saita Phys. Fluid **11** (1999) 786

Modeling of front curvature

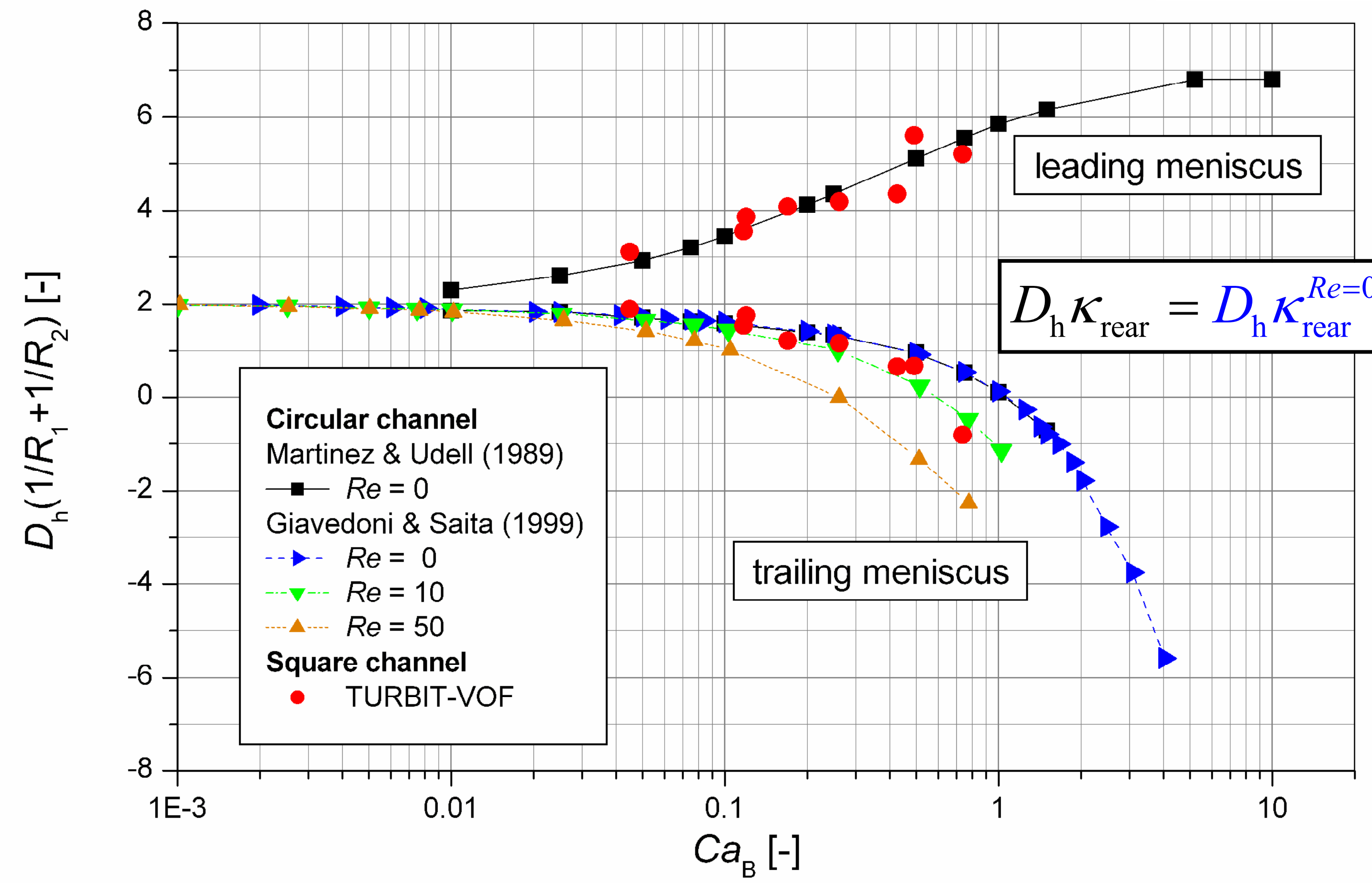
- The non-dimensional front curvature depends on Ca_B only



$$D_h \kappa_{front} = 7.07 - \frac{7.07 - 2.121}{1 + 2.961 Ca_B^{0.916}}$$

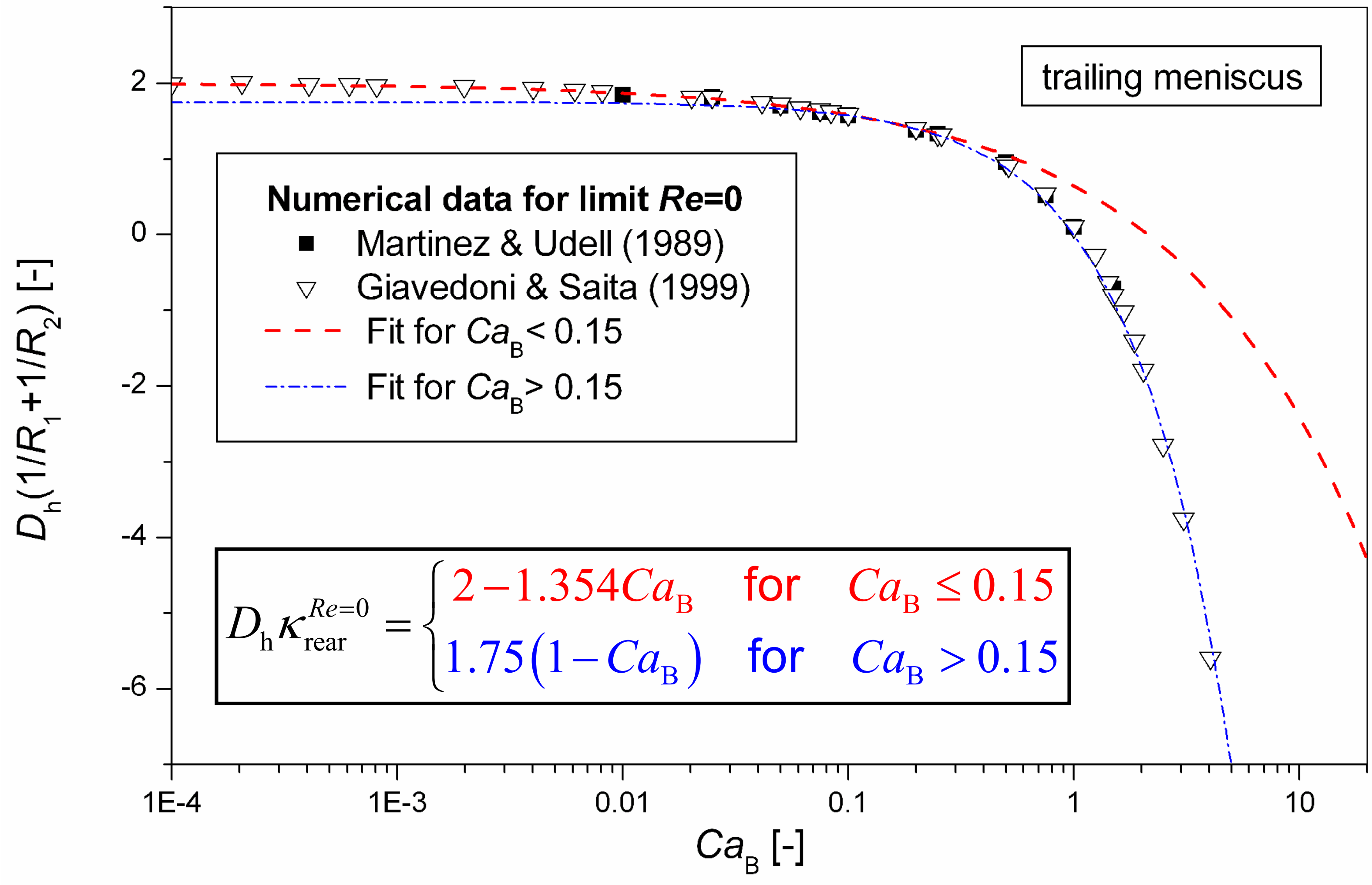
Modeling of rear curvature

- The non-dimensional rear curvature depends on Ca_B and Re_B
- It is modeled as the sum of two contributions: $\kappa_\mathrm{rear} = \kappa_\mathrm{rear}^{Re=0} + \kappa_\mathrm{rear}^{Re>0}$



$$D_\mathrm{h}\kappa_\mathrm{rear} = D_\mathrm{h}\kappa_\mathrm{rear}^{Re=0} + D_\mathrm{h}\kappa_\mathrm{rear}^{Re>0}$$

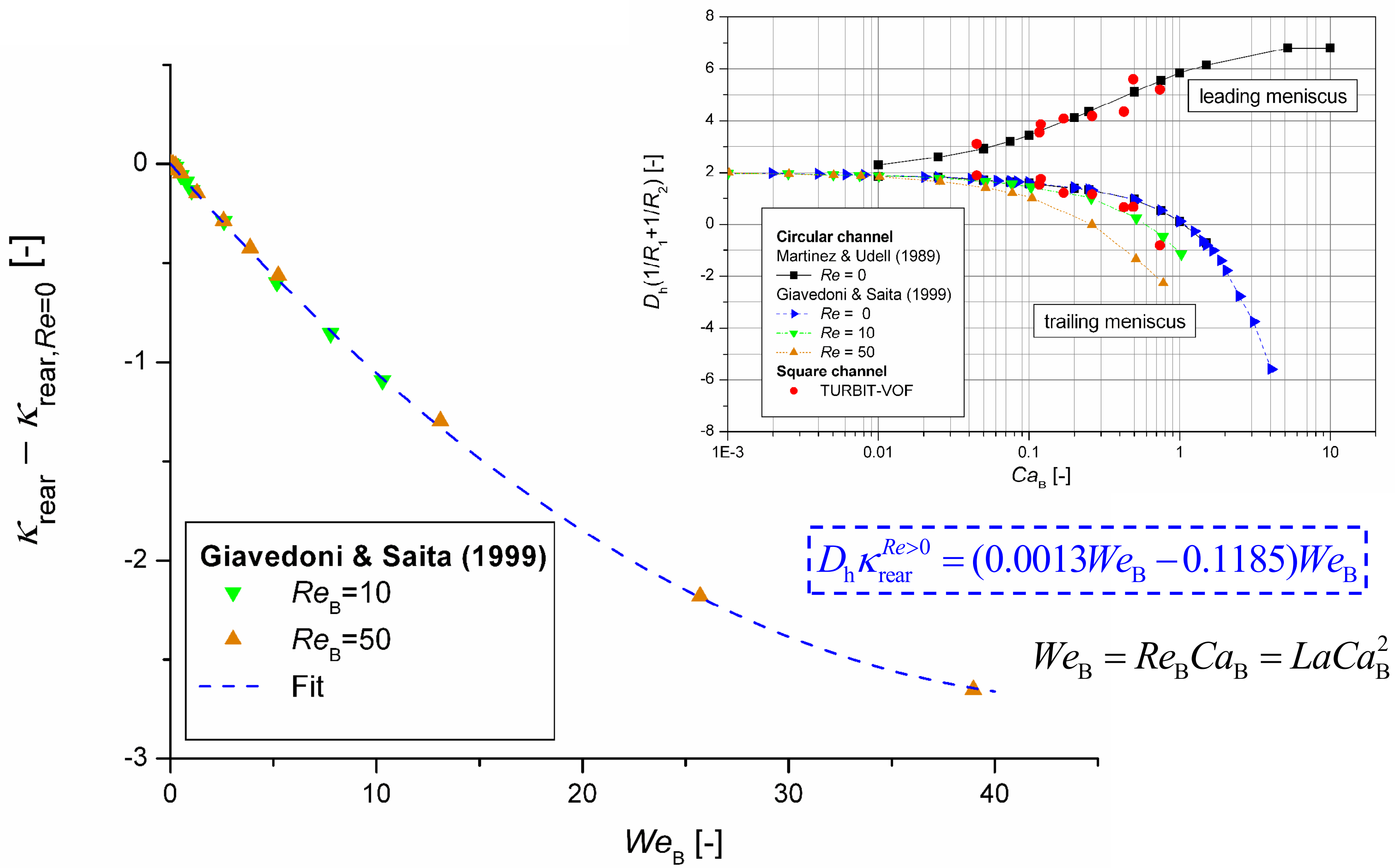
Rear curvature in limit $Re_B = 0$



Numerical data for limit *Re*=0
- ■ Martinez & Udell (1989)
- ▽ Giavedoni & Saita (1999)
- Fit for $Ca_B < 0.15$
- Fit for $Ca_B > 0.15$

$$D_h \kappa_{\mathrm{rear}}^{Re=0} = \begin{cases} 2 - 1.354 Ca_B & \text{for} \quad Ca_B \le 0.15 \\ 1.75(1 - Ca_B) & \text{for} \quad Ca_B > 0.15 \end{cases}$$

Rear curvature for $Re_B > 0$



$$D_h \kappa_{rear}^{Re>0} = (0.0013 We_B - 0.1185) We_B$$

$$We_B = Re_B Ca_B = La Ca_B^2$$

Closure of the model

Karlsruher Institut für Technologie

- At this stage, the model is not closed since the front and rear curvatures depend on Ca_B which involves the unknown bubble velocity

$$Ca_\mathrm{B} = \frac{\mu_\mathrm{L} U_\mathrm{B}}{\sigma}$$

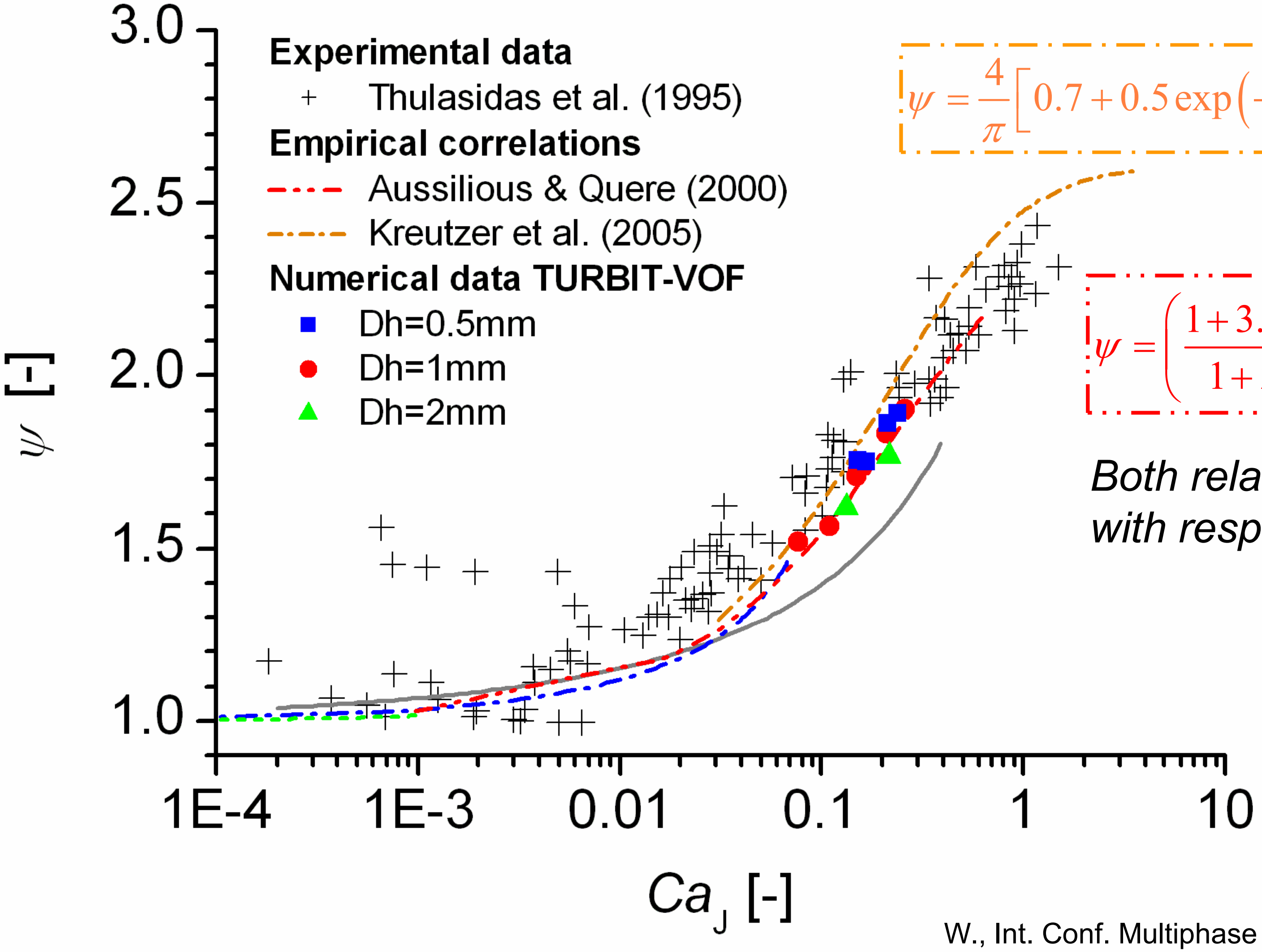
- As a remedy we relate U_B to the total superficial velocity J_total

$$\psi = \frac{U_\mathrm{B}}{J_\mathrm{total}} \qquad \rightarrow \qquad Ca_\mathrm{B} = \frac{U_\mathrm{B}}{J_\mathrm{total}} \frac{\mu_\mathrm{L} J_\mathrm{total}}{\sigma} = \psi Ca_\mathrm{J}$$

- The ratio ψ is obtained by fitting experimental and numerical data

$$\psi = \psi(Ca_\mathrm{J})$$

Relation between ψ and Ca_J



$$\psi = \frac{4}{\pi}\left[0.7+0.5\exp\left(-2.25\psi^{0.445}Ca_J^{0.445}\right)\right]^{-2}$$

$$\psi = \left(\frac{1+3.33\psi^{2/3}Ca_J^{2/3}}{1+2\psi^{2/3}Ca_J^{2/3}}\right)^{2}$$

Both relations are implicit with respect to ψ

W., Int. Conf. Multiphase Flow, Tampa, USA, 2010

Summary of pressure drop model

Input: $\rho_L, \mu_L, \sigma, g, D_\mathrm{h}, L_\mathrm{uc}, J_\mathrm{L}, J_\mathrm{G} \quad \rightarrow \quad \beta, La, Ca_\mathrm{J}$

$$\rightarrow \quad \psi = \left(\frac{1 + 3.33\psi^{2/3} Ca_\mathrm{J}^{2/3}}{1 + 2\psi^{2/3} Ca_\mathrm{J}^{2/3}} \right)^2$$

Model:

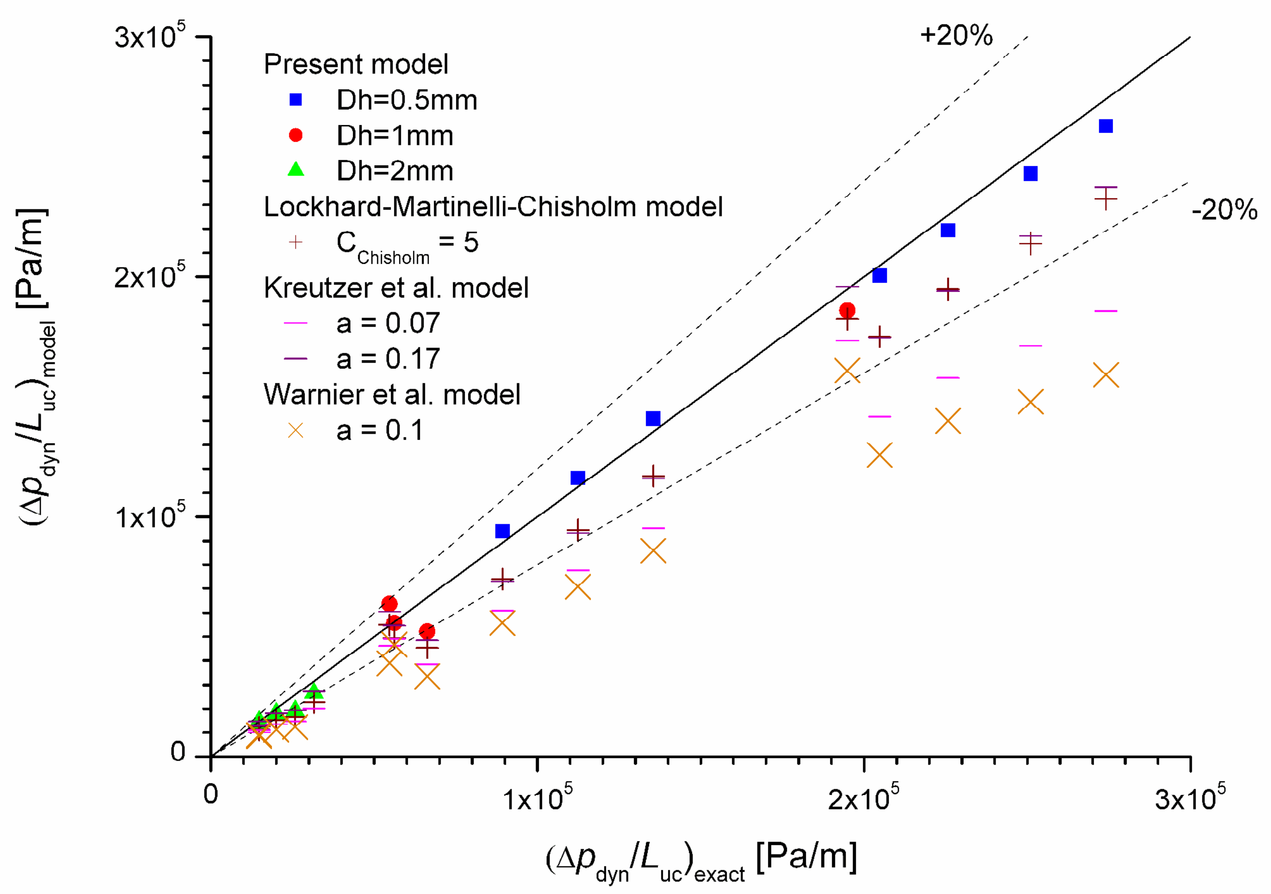
$$\frac{\Delta P_\mathrm{uc}}{L_\mathrm{uc}} = \frac{C_\mathrm{f}}{2} \frac{\mu_\mathrm{L} J_\mathrm{total}}{D_\mathrm{h}^2} \left[1 - 1.5\beta(1-\beta) - \beta^2 \right] + \left(D_\mathrm{h}\kappa_\mathrm{rear}^{Re=0} + D_\mathrm{h}\kappa_\mathrm{rear}^{Re>0} - D_\mathrm{h}\kappa_\mathrm{front} \right) \frac{D_\mathrm{h}}{L_\mathrm{uc}} \frac{\sigma}{D_\mathrm{h}^2}$$

$$D_\mathrm{h}\kappa_\mathrm{rear}^{Re=0} = \begin{cases} 2 - 1.354\psi Ca_\mathrm{J} & \text{for} \quad \psi Ca_\mathrm{J} \le 0.15 \\ 1.75(1 - \psi Ca_\mathrm{J}) & \text{for} \quad \psi Ca_\mathrm{J} > 0.15 \end{cases}$$

$$D_\mathrm{h}\kappa_\mathrm{rear}^{Re>0} = (0.0013\psi^2 La Ca_\mathrm{J}^2 - 0.1185)\psi^2 La Ca_\mathrm{J}^2 \quad \text{for} \quad \psi^2 La Ca_\mathrm{J}^2 \le 40$$

$$D_\mathrm{h}\kappa_\mathrm{front} = 7.07 - \frac{7.07 - 2.121}{1 + 2.961\psi^{0.916} Ca_\mathrm{J}^{0.916}}$$

Comparison of pressure drop models



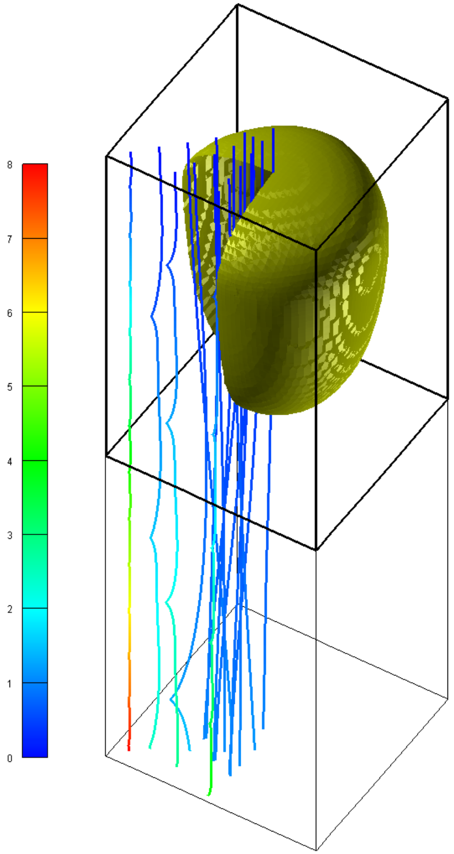
- The new model is in good agreement with DNS data (not surprising) → compare model with experimental pressure drop data

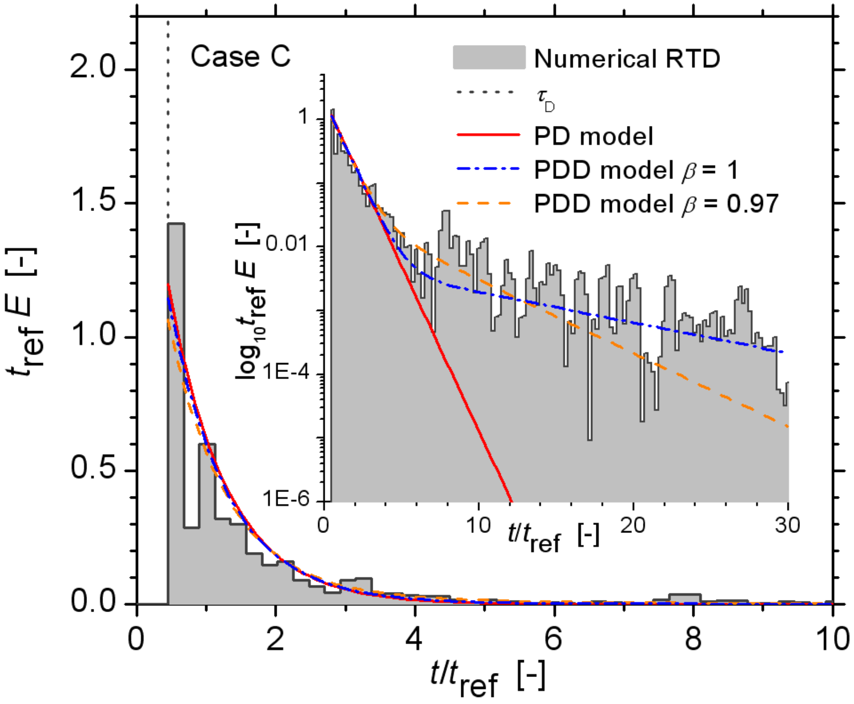
Residence time distribution

- Liquid flows in micro-channels are usually laminar and species diffusivities are usually low (high Schmidt number)
- The RTD is therefore significantly affected by the non-uniform velocity distribution → the RTD is rather broad
  - Conventional RTD models (PFR, CSTR, axial-dispersed plug flow model) are often not appropriate
  - Influence of channel shape on diffusion-free RTD (analytical)
    W., CES **65** (2010) 3499, Erdogan & W., CEJ **227** (2013) 158
- Segmented flow (Taylor flow) narrows the RTD (A. Günther)

RTD in Taylor flow

- Evaluation of the diffusion-free RTD from simulation results by tracking a set of virtual particles and recording the time the particle needs to travel a certain axial distance

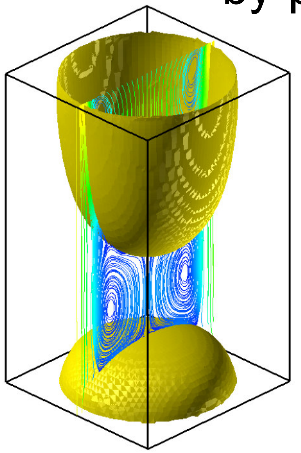


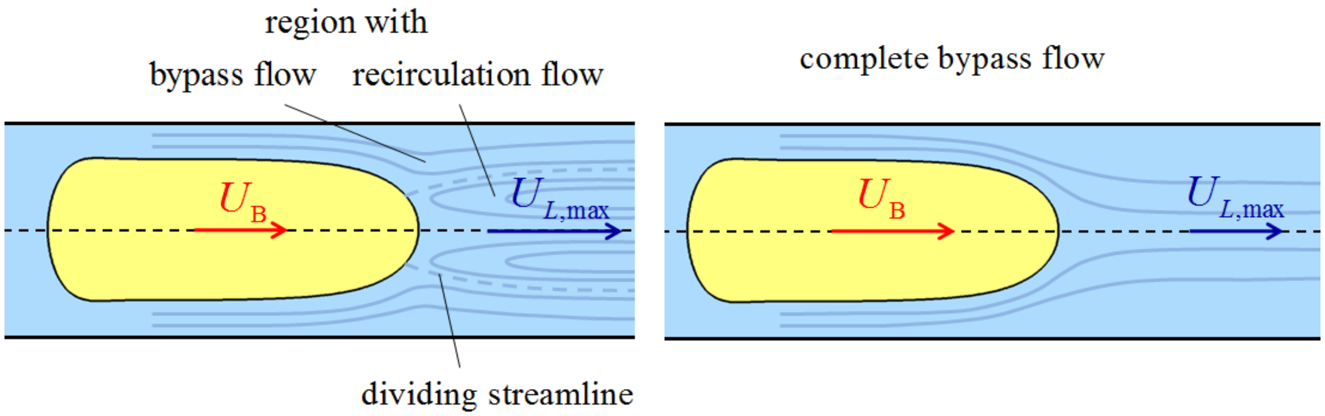


Erdogan, W., Soyhan, **200-202** CEJ (2012) 380

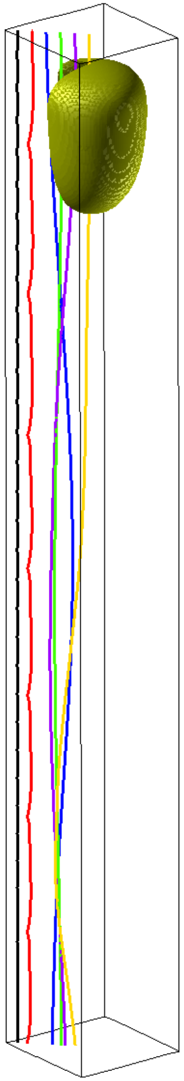
RTD in Taylor flow

- RTD of one unit cell be modeled as PFR-CSTR in series
- Determining the RTD of multiple unit cells by convoluting the single unit-cell RTD fails
  - Reason: the liquid in a unit cell consists of two regions: by-pass flow and recirculation flow (Thulasidas et al. 1995)





  - In absence of diffusion there is no exchange across the dividing streamline → neighboring units cells are not independent
- The size of both regions depends on $\psi = U_B / J_{total}$
  for rectangular channels see Kececi, W., Onea, Soyhan; Catalysis Today **147S** (2009) S125
- A reliable RTD model should account for this

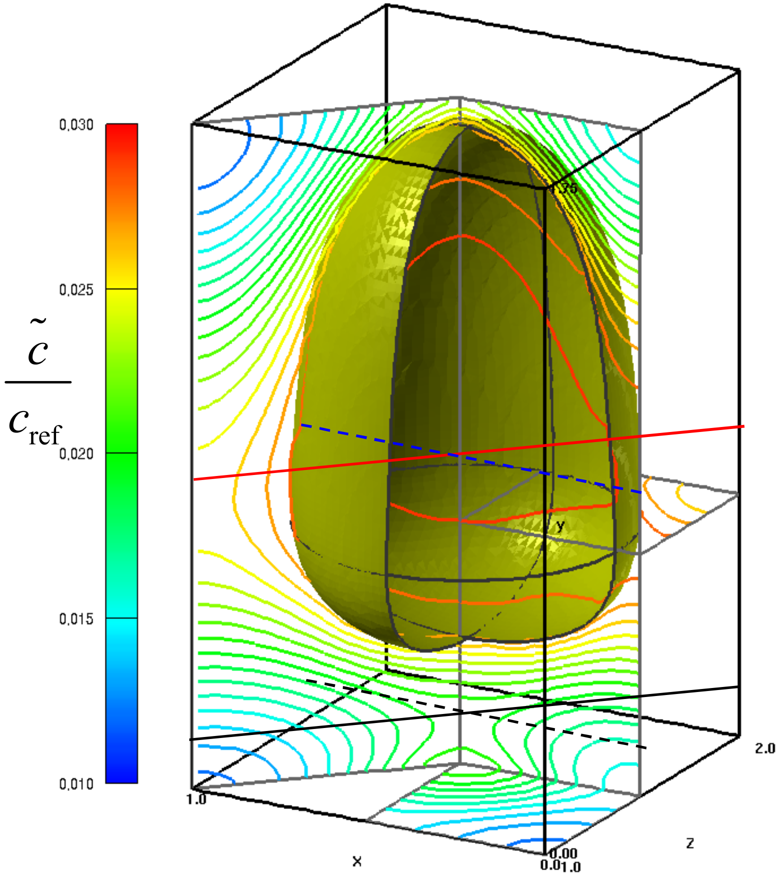


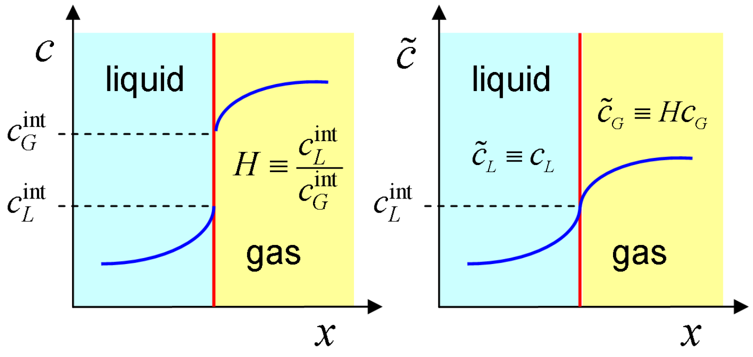
Outline

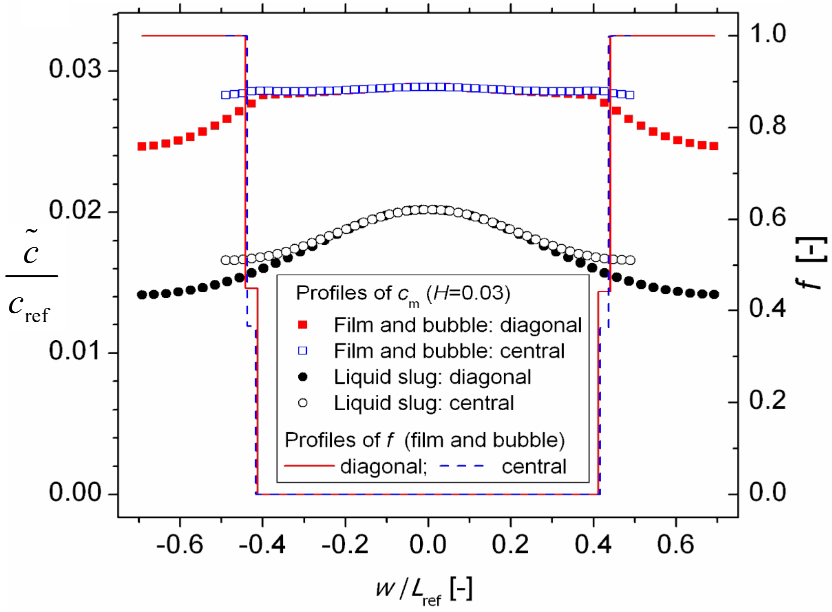
- Introduction
- Computational fluid dynamics in micro process engineering
  - Status and developments
- Taylor flow in square capillaries
  - Numerical method and computational setup
  - Insight by scale-resolving simulations
  - Development of engineering models
    - Pressure drop
    - Residence time distribution
- Short survey on further ongoing projects in the group
- Summary

Gas-liquid mass transfer

- Transient simulations ("<u>qualitative</u>") $Sc_L = \nu_L / D_L = 0.8$, $H = 0.03$
  Onea et al. Chem. Eng. Sci. 64 (2009) 1416 –1435

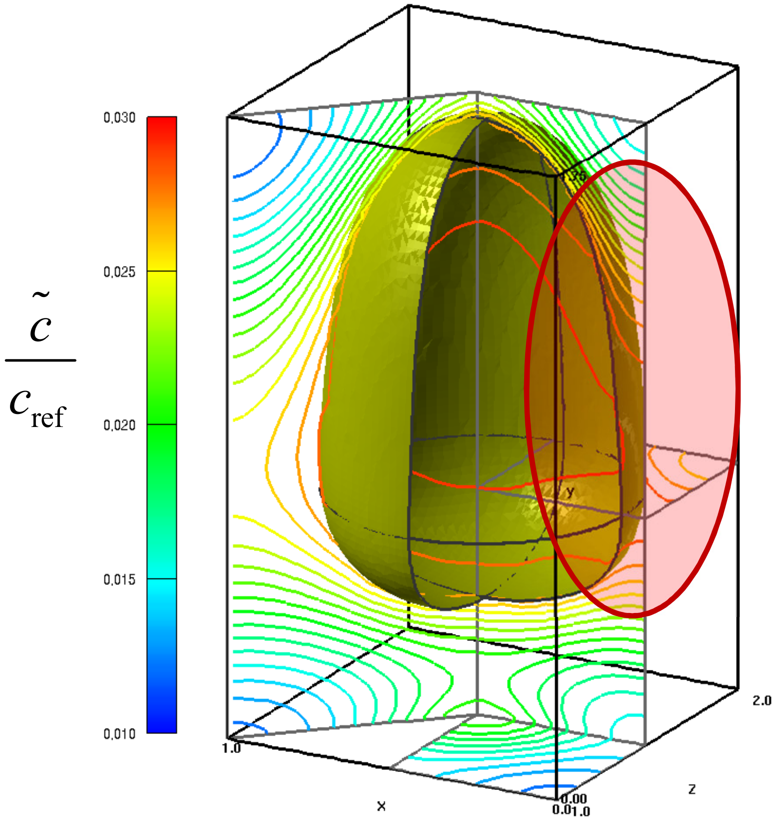




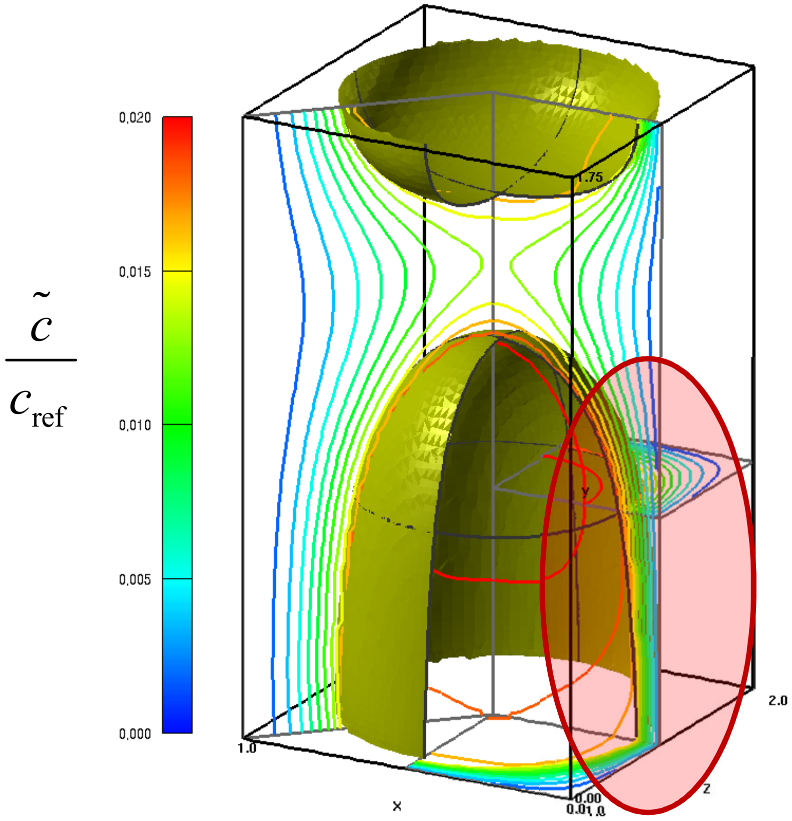


Mass transfer and chemical reaction

- Without chemical reaction
- Fast heterog. reaction (1^{st} o.)



Short bubbles are more efficient



Long bubbles are more efficient

Scale separation in mass transfer

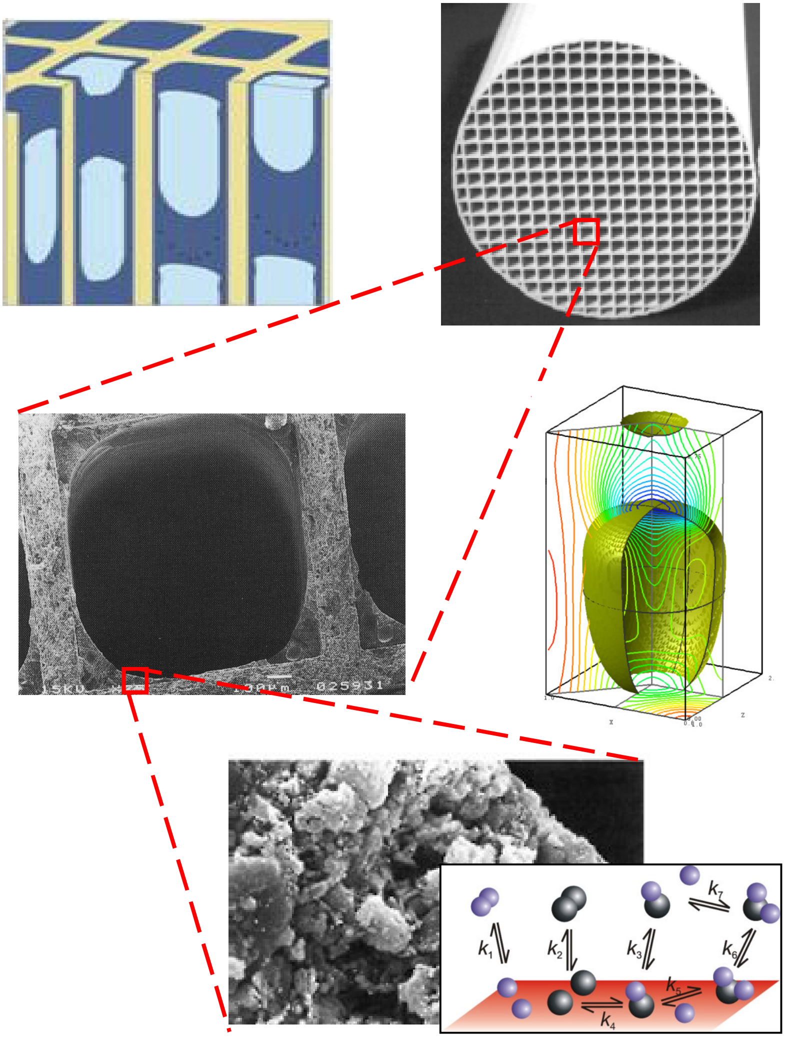
- Ratio of the smallest scales in the concentration and velocity field and the thickness of the boundary layers

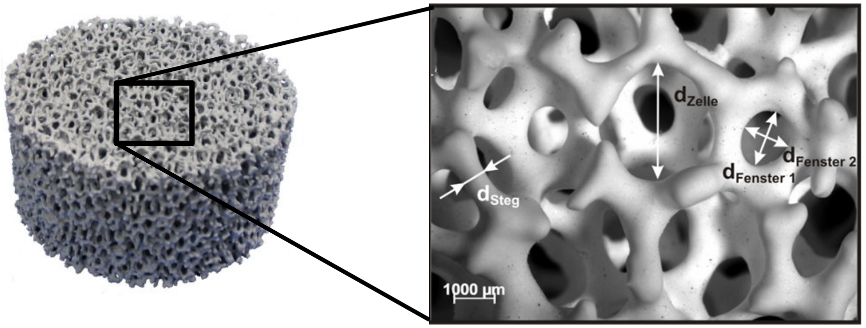
$$\frac{\lambda_{\mathrm{c}}}{\lambda_{\mathrm{u}}} \propto \frac{(\nu D^2/\varepsilon)^{1/4}}{(\nu^3/\varepsilon)^{1/4}} \propto \sqrt{\frac{D}{\nu}} = \frac{1}{\sqrt{Sc}} \qquad \frac{\delta_{\mathrm{c}}}{\delta_{\mathrm{u}}} \propto \frac{L/\sqrt{Pe}}{L/\sqrt{Re}} = \frac{1}{\sqrt{Sc}}$$

- Liquids: $Sc = O(1000) \rightarrow$ the grid required to resolve all scales in the concentration field is 30 times finer than for the velocity field (in 3D this corresponds to 30^3 = 27 000)
- This makes numerical methods that use the same grid for the velocity and concentration field very inefficient
  $\Rightarrow$ use of a hierarchical grid, i.e. a finer grid for the concentration field than for the velocity field (PhD C. Falconi)

Helmholtz Alliance „Energy efficient chemical multiphase processes"

- **Scale resolving simulations of catalytic multi-phase flows in structured reactors**
    - Oxidation of isobutane
    - Hydrogenation of nitrobenzene
- Single channel of a monolith reactor
    - Coupling TURBIT-VOF / DETCHEM
- Portion of a solid sponge
    - Phase field simulations (OpenFOAM)

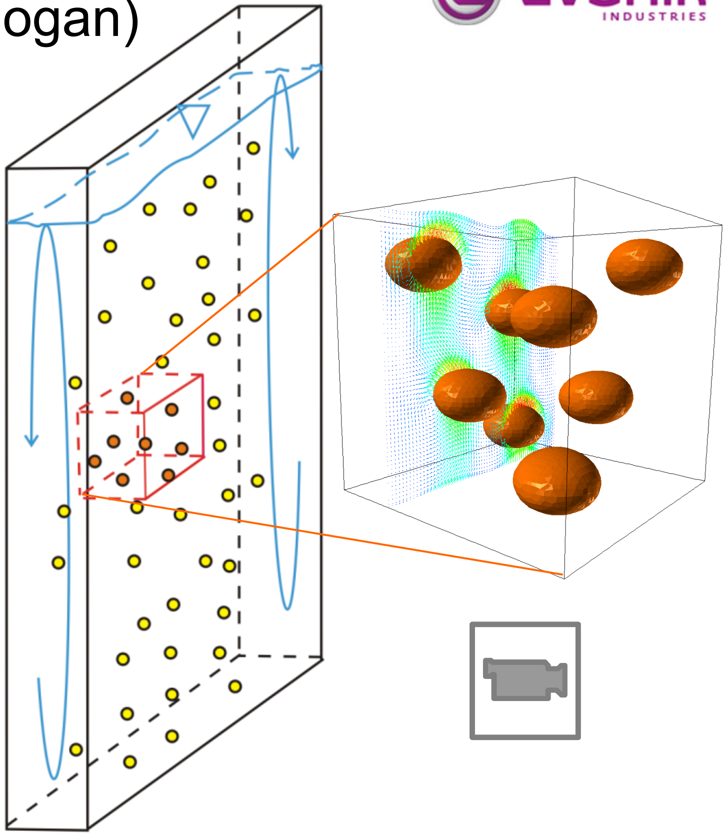




DNS of bubble swarm flows

GEFÖRDERT VOM
Bundesministerium
für Bildung
und Forschung

- BMBF Project “Multiscale Modelling of Multiphase Reactors”
  - Development of scale-up strategies that will allow a model based design of industrial scale multiphase reactors
- Contributions of KIT (PhD project of S. Erdogan)
  - Investigate pseudo-turbulence in bubble swarm flows by DNS
  - Evaluation of all terms in the transport equation for liquid phase turbulent kinetic energy from DNS data
  - Analyze, assess and improve engineering models for bubble-induced turbulence in two-fluid model
  - Implementation of improved models in OpenFOAM, validation by experiments of project partners



Conclusions

- High potential of Taylor flow for intensification of heterogeneously catalyzed gas-liquid processes in microreactors
- Complicate interaction between two-phase flow hydrodynamics, transport of mass and heat, and chemical reaction
- Understanding and quantification of this non-linear interaction (which involves various length and time scales) is a key issue toward the design and optimization of multi-phase micro reactors
- Detailed numerical investigations provide a promising tool for understanding the phenomena and for developing engineering models
- Current status of interface resolving numerical simulation methods
  - Hydrodynamics of two-phase flow including bubble and drop formation ✓
  - *Coalescence phenomena* 👓
  - *Mass transfer (realistic Schmidt numbers Sc* = 1000*)* 👓
  - *Interfacial transport of soluble and insoluble surfactants* 👓
  - *Coupling of two-phase flow and transport with detailed chem. kinetics* 👓

Acknowledgements

- PhD students
  - W. Sabisch (2000)
  - B. Ghidersa (2004)
  - M. Ilić (2005)
  - A. Onea (2007)
  - X. Cai, C. Falconi, S. Erdogan, M. Woo
- Erasmus students from Sakarya University (Turkey)
  - F. Özkan (2006)
  - Ö. Keskin (2007)
  - M. Öztaskin (2007)
  - S. Kececi (2008)
  - A. Boran (2010)

- Funding

HELMHOLTZ
GEMEINSCHAFT

DFG Deutsche Forschungsgemeinschaft

Transport processes at fluidic interfaces
DFG SPP 1506

GEFÖRDERT VOM
Bundesministerium
für Bildung
und Forschung

- Cooperation

EVONIK
INDUSTRIES

TECHNISCHE
UNIVERSITÄT
DRESDEN

TECHNISCHE
UNIVERSITÄT
DARMSTADT

HZDR

HELMHOLTZ
ZENTRUM DRESDEN
ROSSENDORF

TUHH
Institut für
Mehrphasenströmungen
ims