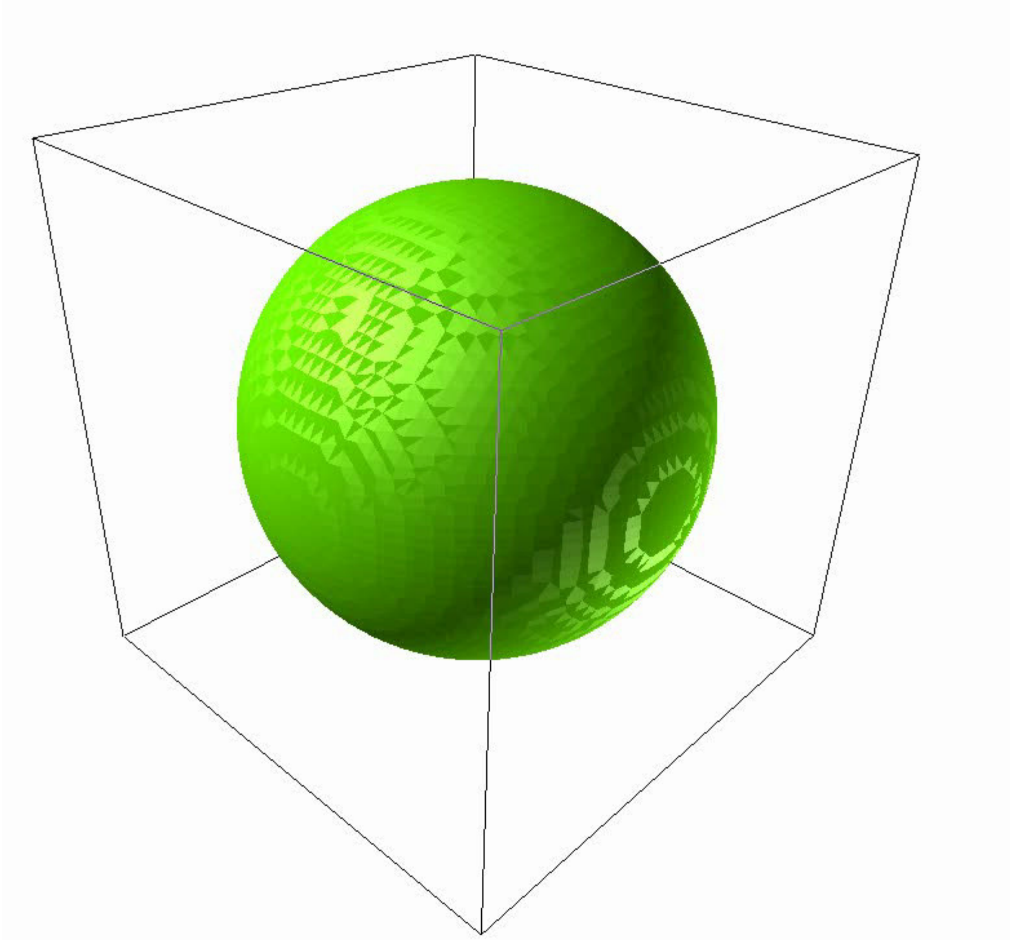
Detailed numerical investigations of two-phase flow and transport phenomena in narrow channels



Dr.-Ing. Martin Wörner

Institut für Kern- und Energietechnik

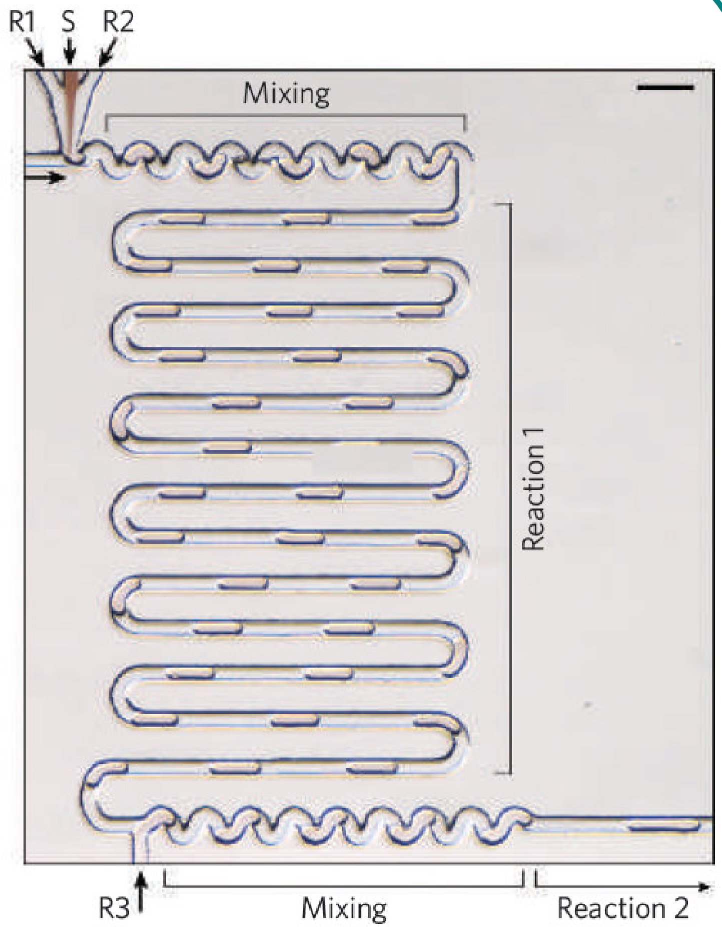
Opening Workshop Helmholtz Research School Energy-Related Catalysis

Karlsruhe Institute of Technology
November 17, 2010

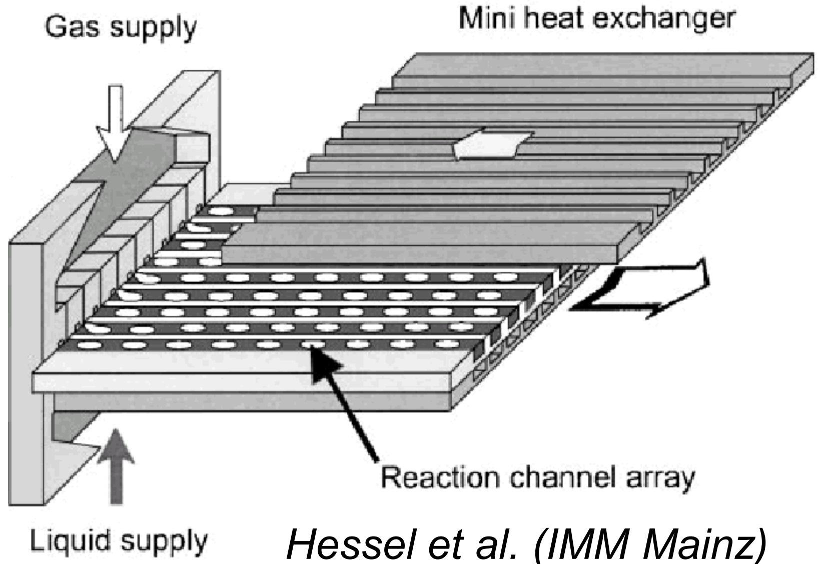
Outline

- Introduction
  - Multiphase micro reactors
  - Interaction between flow, transport and reaction
- Numerical simulation method
- Results
  - Hydrodynamics
  - Mass transfer
  - Chemical reaction
- Conclusions and outlook

Multiphase micro reactors

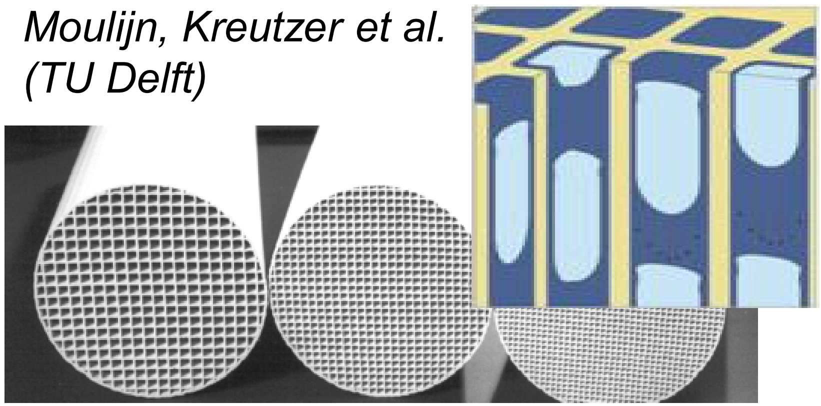


Ismagilov et al. (Univ. Chicago)



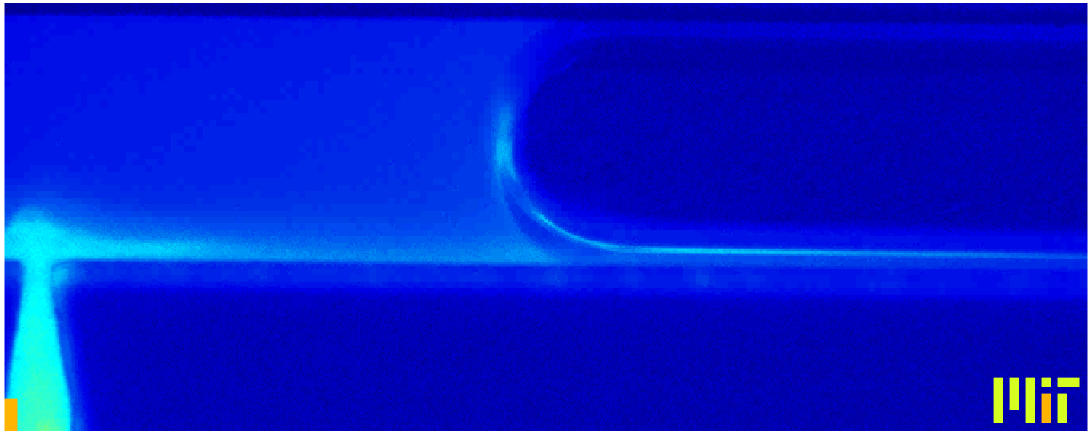
Hessel et al. (IMM Mainz)

Moulijn, Kreutzer et al. (TU Delft)



Advantages of Taylor flow

- Good mixing of species within the bubble
- Large interfacial area per unit volume and thin liquid film between bubble and wall $\Rightarrow$ efficient heat and mass transfer
- Axial segmentation of liquid $\Rightarrow$ reduced axial dispersion
- Recirculation in liquid slug $\Rightarrow$ good mixing in liquid slug and wall-normal convective transport in laminar flow



Channel cross section:
400 μm × 280 μm

*Movie of Günther et al. Langmuir **21** (2005) 1547-1555*

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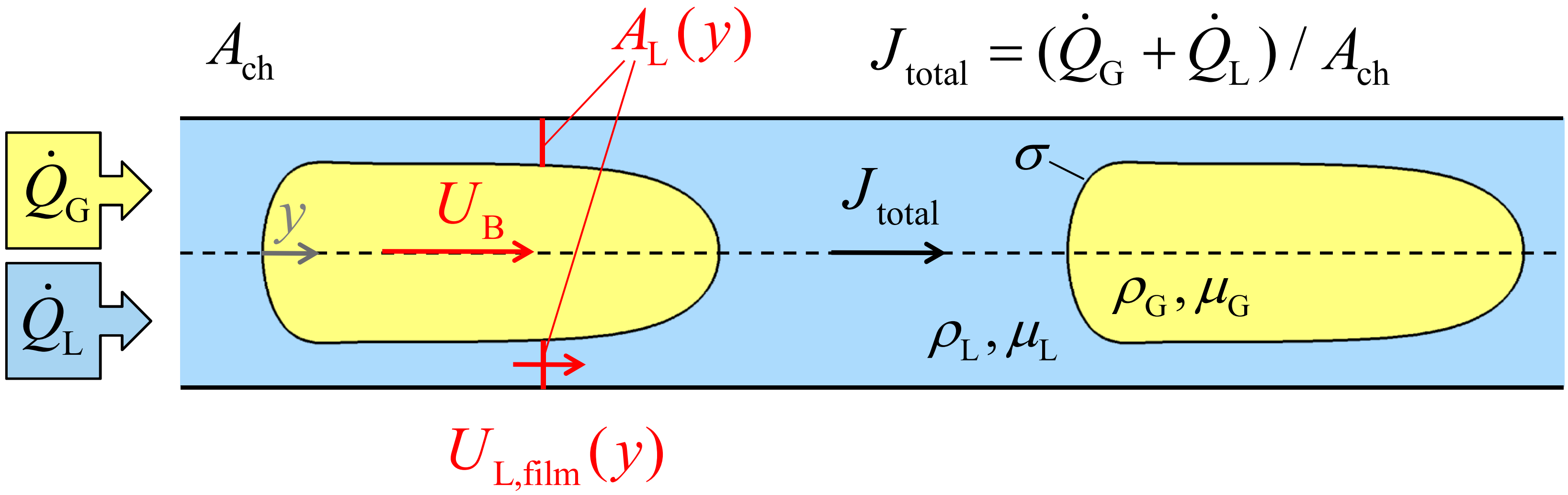
Hydrodynamics

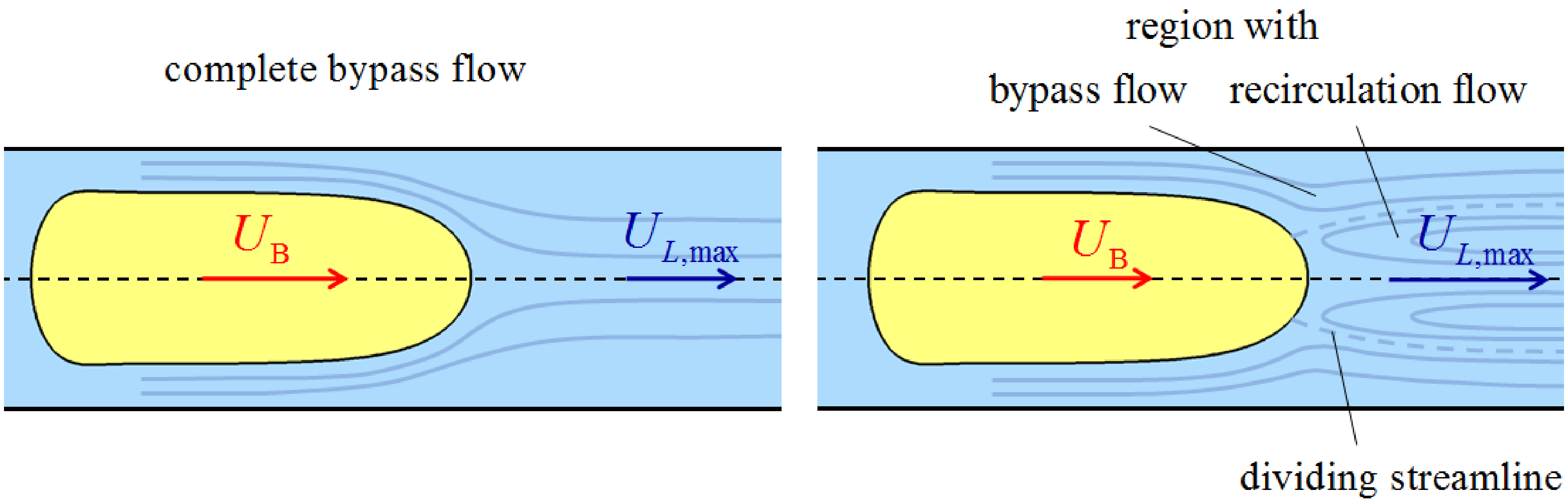


- Bubble velocity U_B is a priori unknown
  - It depends on viscous, capillary, inertial and gravitational forces and is determined by the momentum equations of the two phases
  - The thickness and velocity of the liquid film as well as the volumetric gas content ε_G are closely related to U_B

$$\frac{A_L(y)}{A_{ch}} = \frac{U_B - J_{tot}}{U_B - U_{L,film}(y)} \qquad \varepsilon_G \equiv \frac{V_G}{V_G + V_L} = \frac{\dot{Q}_G}{U_B A_{ch}}$$

Hydrodynamics (cont.)

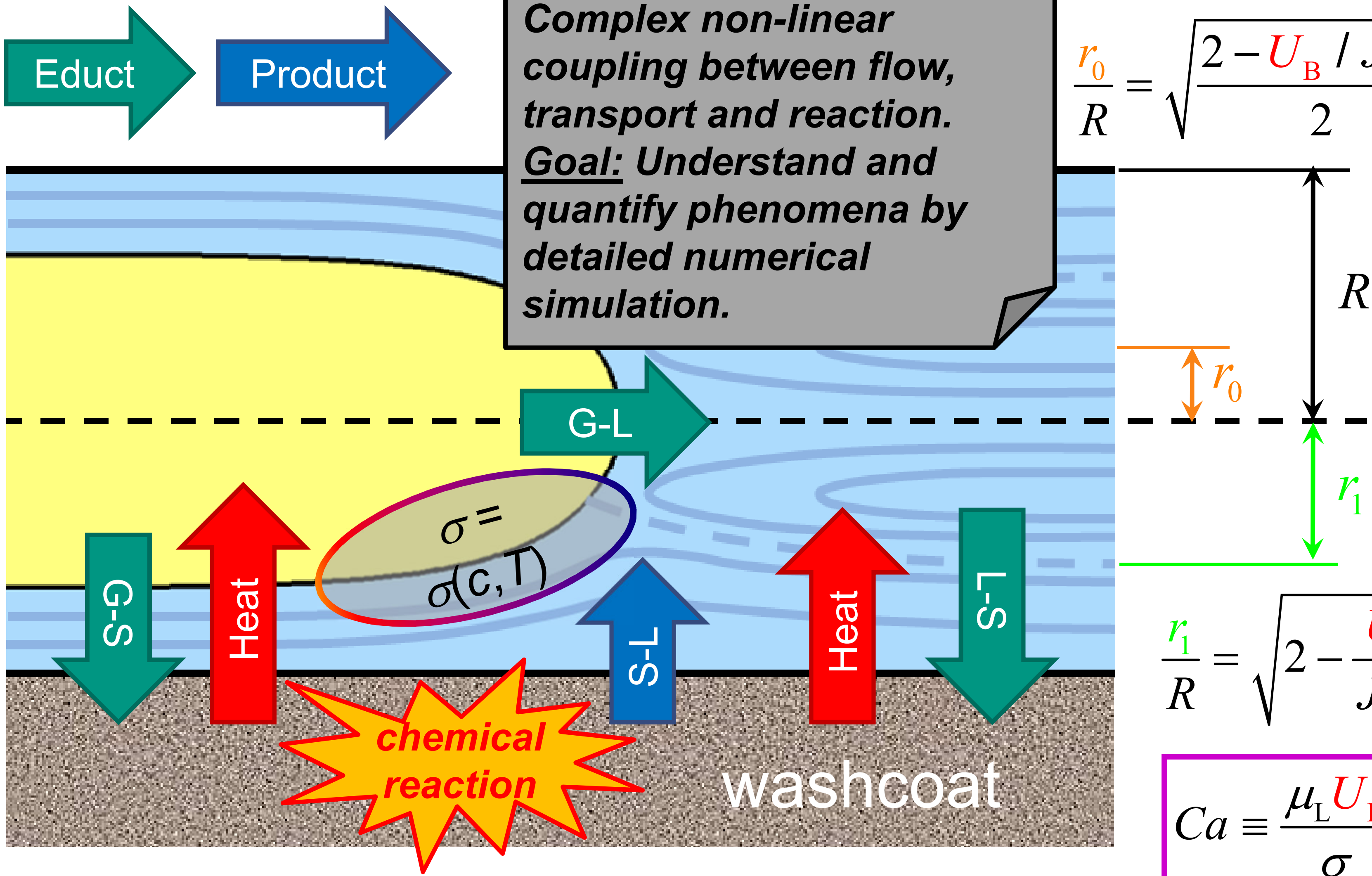
- Sketch of streamlines in moving frame of reference



$$U_{L,\max} = C \cdot J_{\text{total}} \quad (C_{\bigcirc} = 2;\ C_{\square} = 2.096)$$

Condition for bypass flow is	Condition for recirculation flow is
$U_B \geq C \cdot J_{\text{total}}$	$U_B < C \cdot J_{\text{total}}$

Mass transfer and reaction



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

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

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

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

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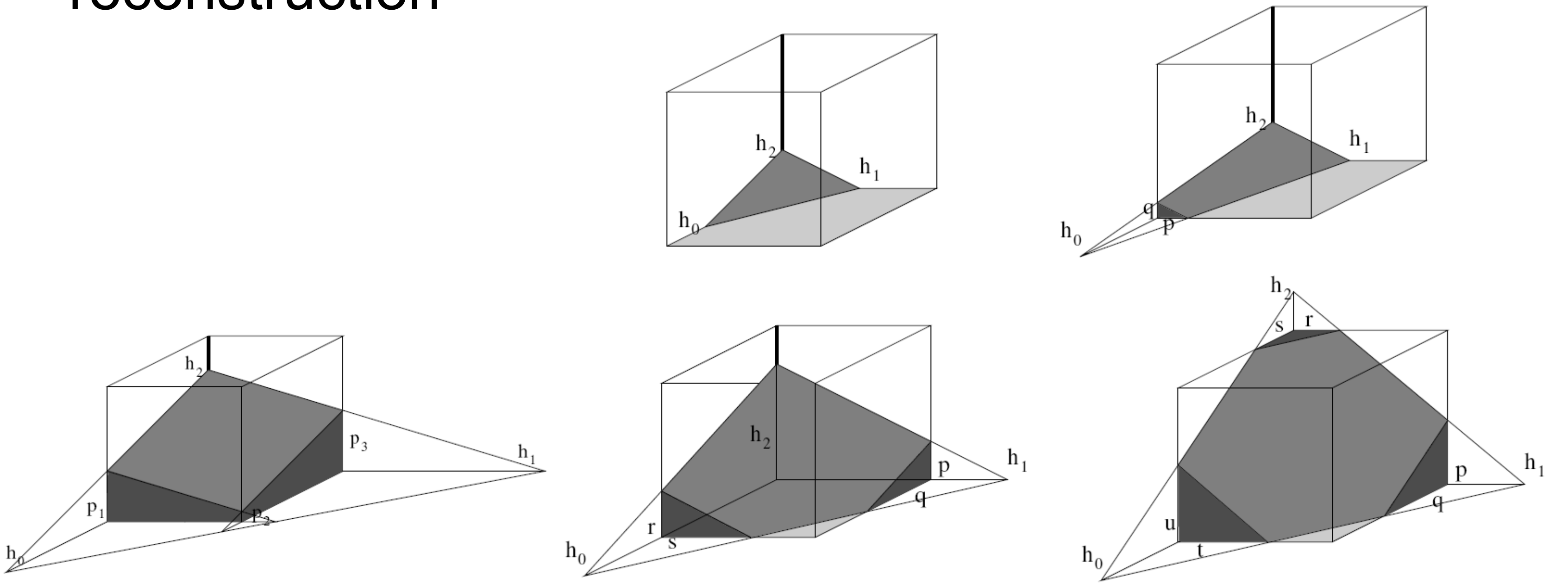
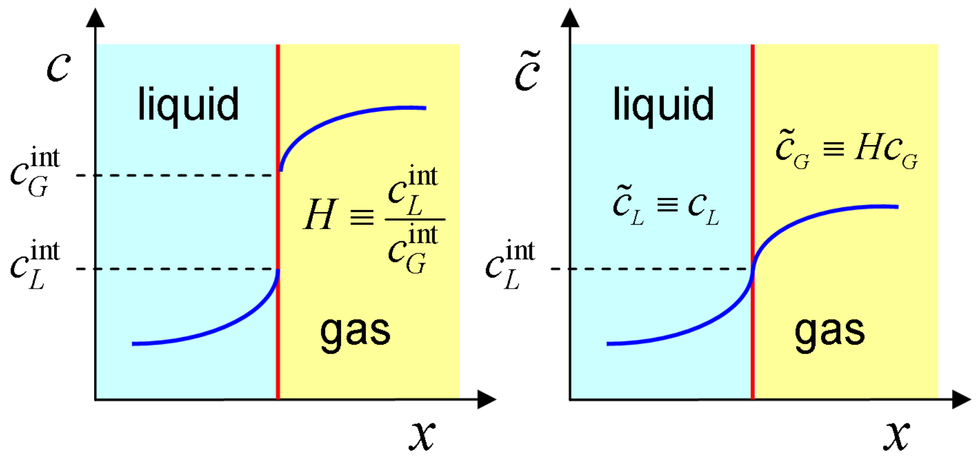
Simulation method*

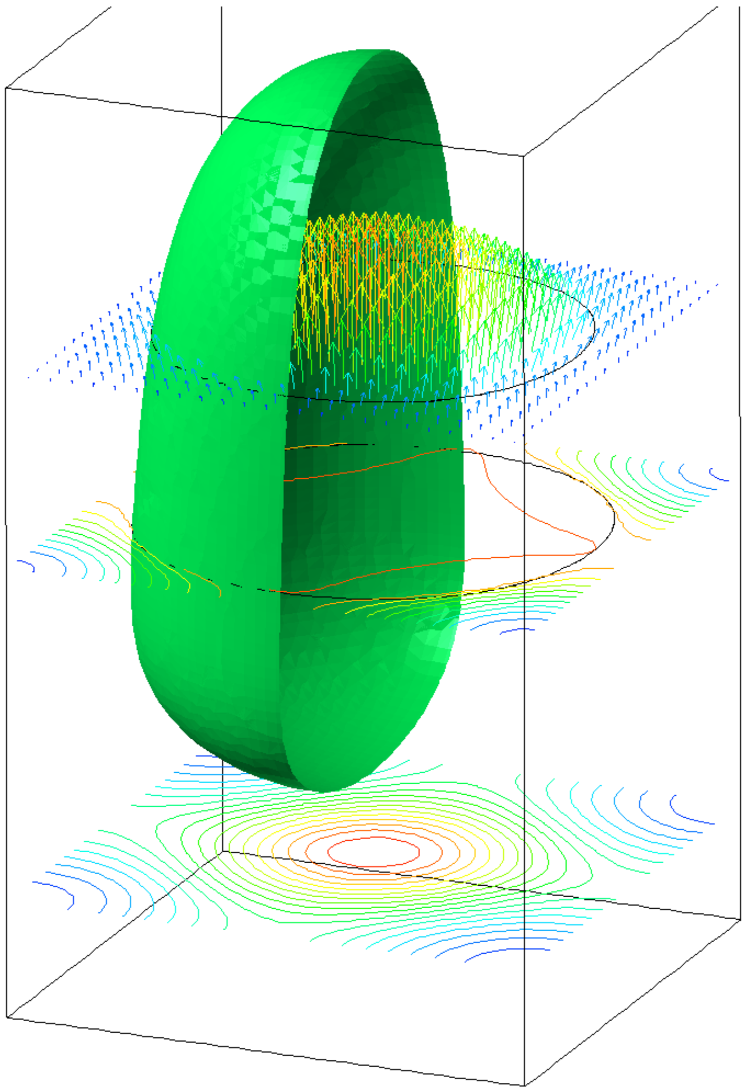
- In-house computer code *Öztaskin et al. Phys. Fluids **21** (2009) 042108
- Navier-Stokes equation in single field formulation with surface tension term for two incompressible immiscible Newtonian fluids with constant physical properties
- Volume-of-fluid method with piecewise linear interface reconstruction



Simulation method* (cont.)

- Solution of single-field concentration equation for an arbitrary number of chemical species
- No feedback of species on hydrodynamics (yet)





*Onea et al. Chem. Eng. Sci. **64** (2009) 1416–1435

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Computed bubble shapes

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

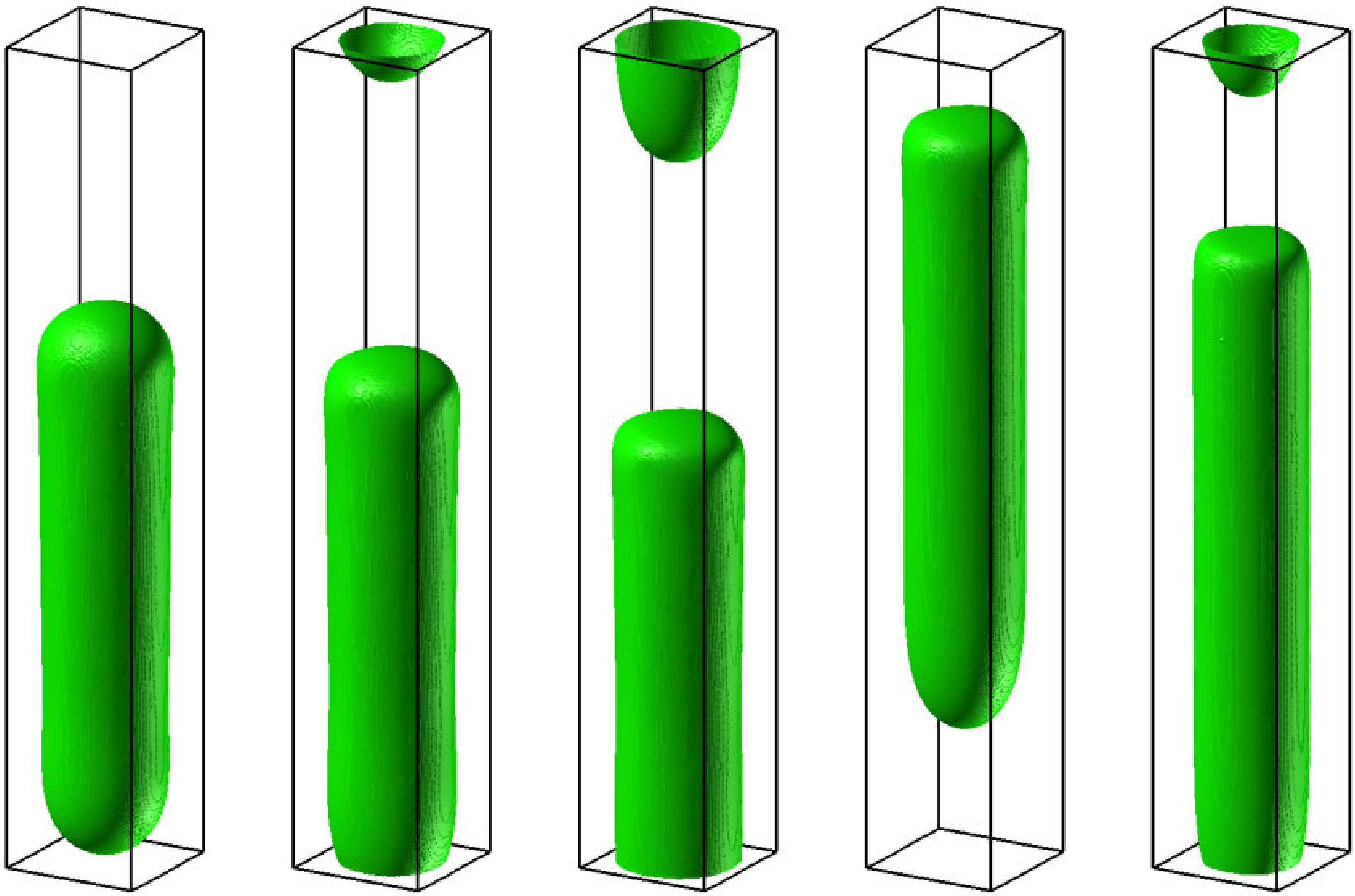
$L_{\text{uc}} = 6\,\text{mm}$

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

$$\frac{Re}{Ca} = \frac{\sigma \rho_{\text{L}} D_{\text{h}}}{\mu_{\text{L}}^2} \equiv La = 27.27$$

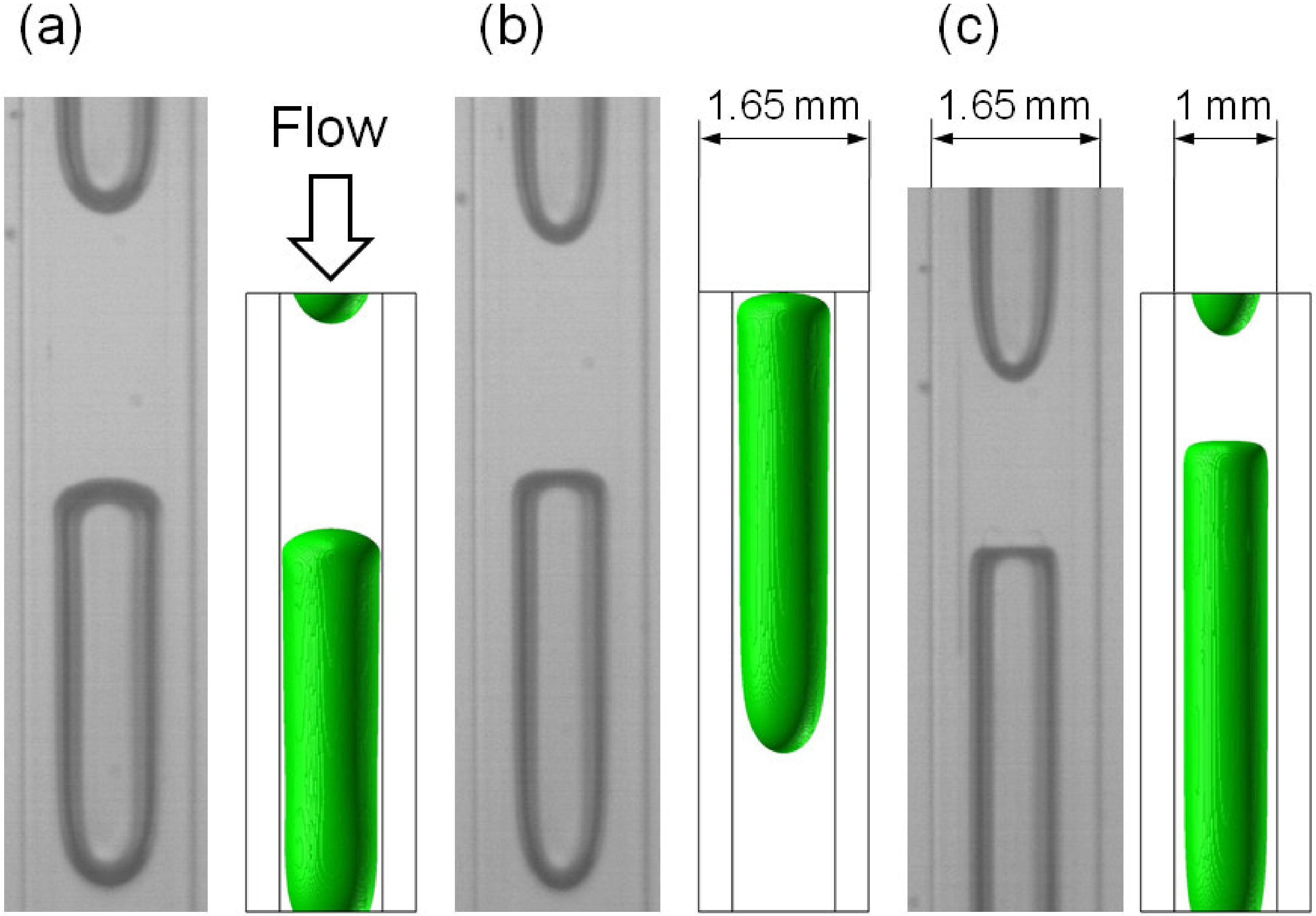
$$Ca \equiv \frac{\mu_{\text{L}} U_{\text{B}}}{\sigma}$$

$$Re \equiv \frac{\rho_{\text{L}} D_{\text{h}} U_{\text{B}}}{\mu_{\text{L}}}$$



Ca =	0.045	0.12	0.17	0.26	0.49
Re =	1.22	3.19	4.64	7.16	13.4

Experimental validation*

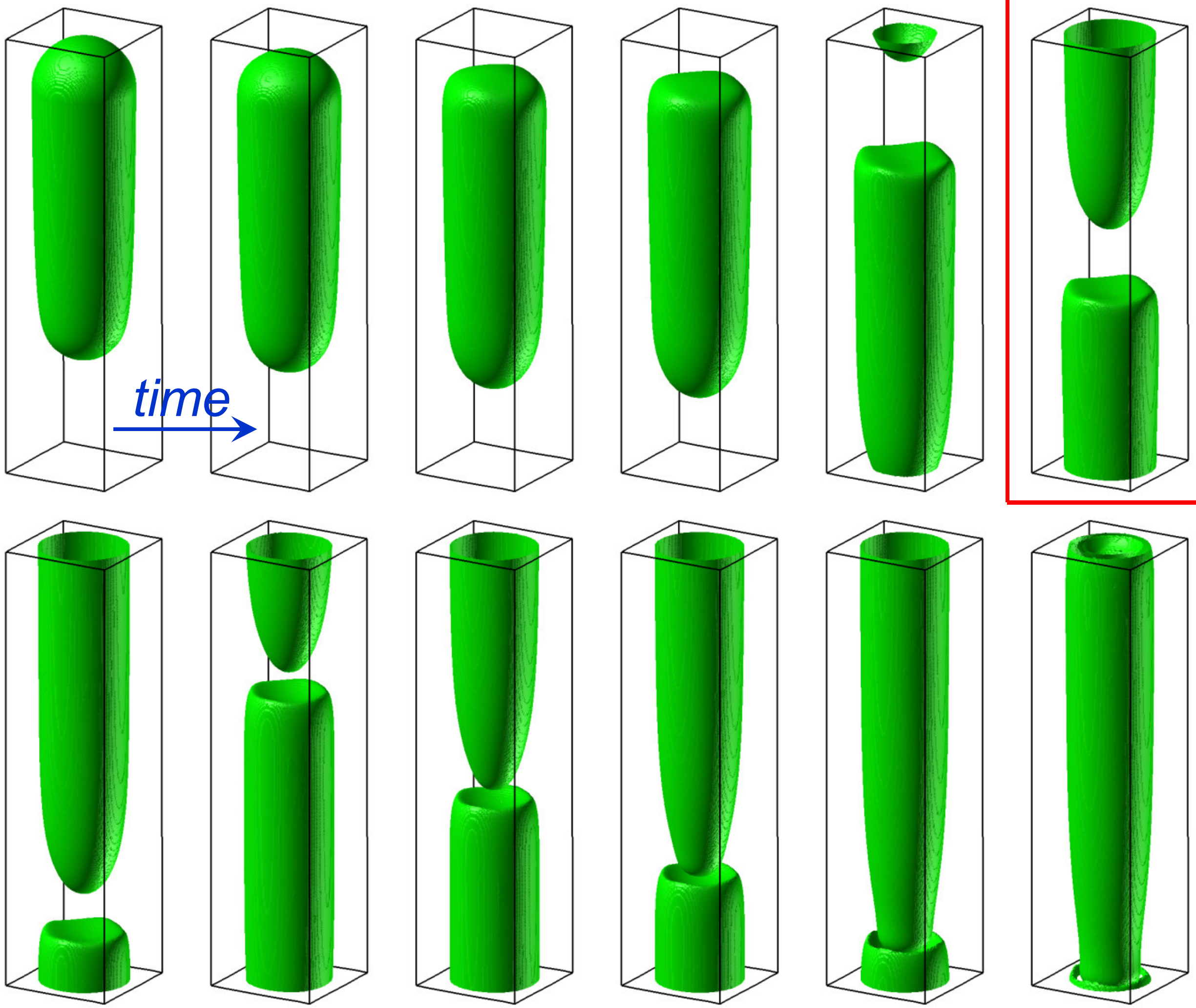


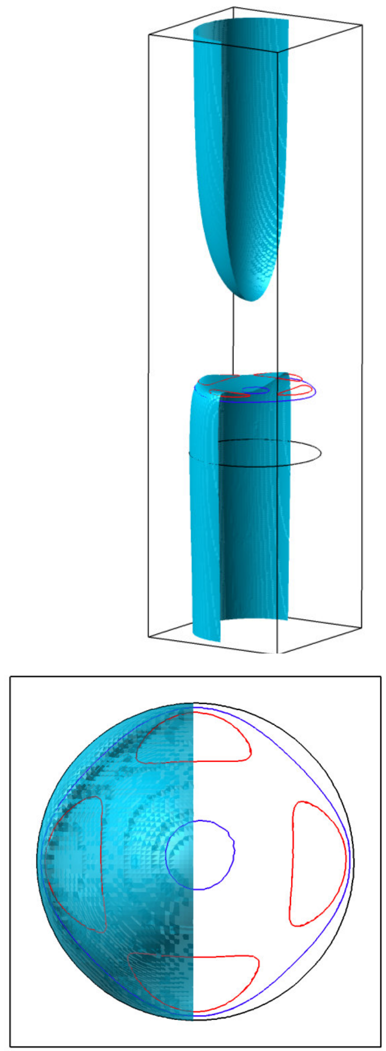
** Experiments by T. Bauer and R. Lange*

TECHNISCHE UNIVERSITÄT DRESDEN

Keskin et al. AIChE J. **56** (2010) 1693–1702

Transition to annular flow





L_{uc} = 4 mm, ε_G = 0.4

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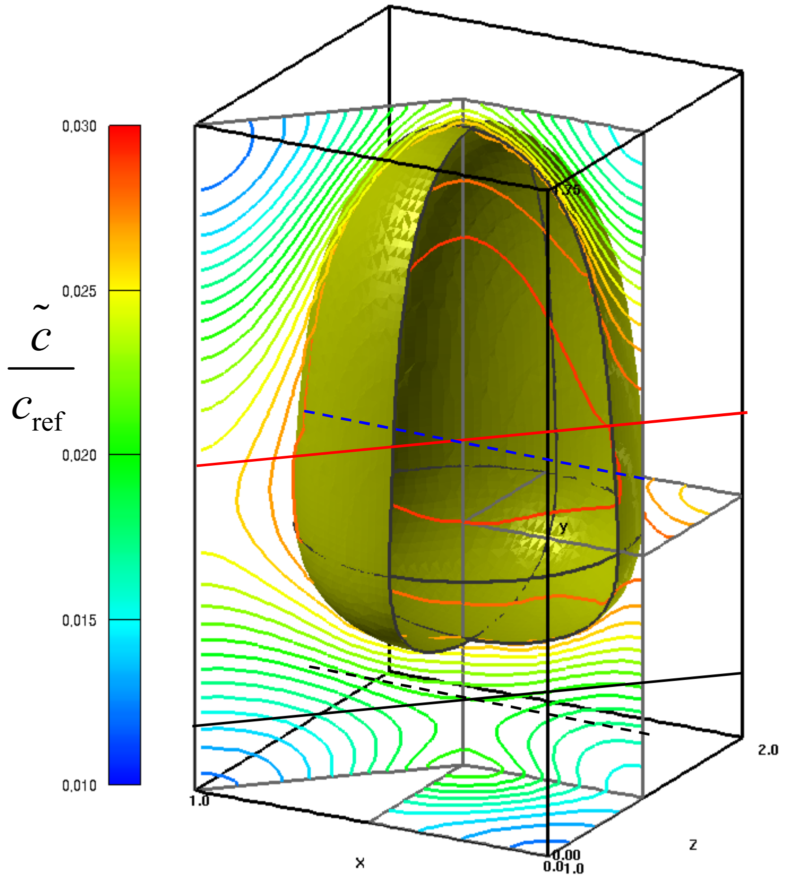
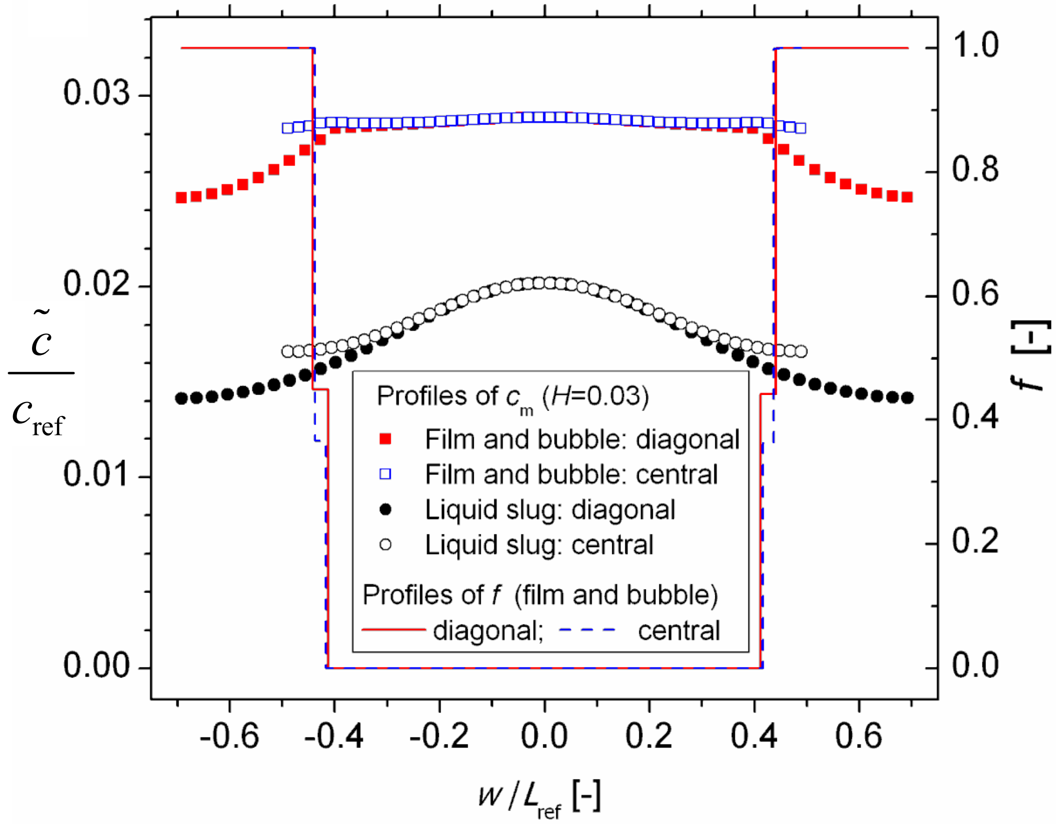
Gas-liquid mass transfer

- Transient simulations ("qualitative") Sc_L=0.8, H=0.03

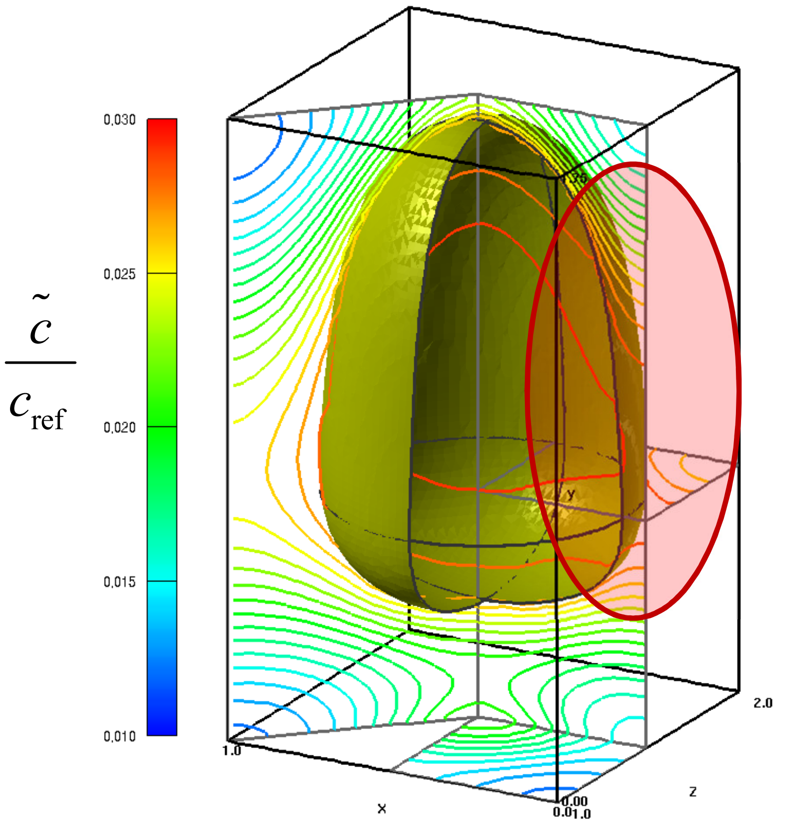
  Onea et al. Chem. Eng. Sci. **64** (2009) 1416 –1435



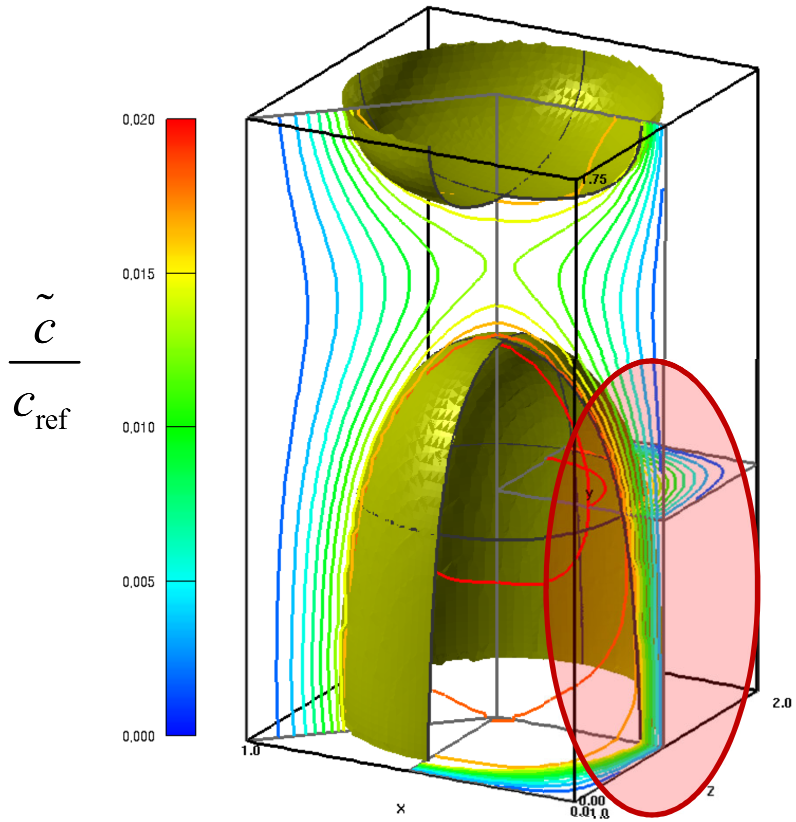


Mass transfer and chemical reaction

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



short bubbles are more efficient



long bubbles are more efficient

Disparity of length scales

- Scale of the smallest structures in the bulk phase
  - Velocity field: Kolmogorov micro-scale $\lambda_{\mathrm{u}} = \left(\nu^3 / \varepsilon\right)^{1/4}$
  - Concentration field: Batchelor scale $\lambda_{\mathrm{c}} = \left(\nu D^2 / \varepsilon\right)^{1/4}$

$$\frac{\lambda_{\mathrm{c}}}{\lambda_{\mathrm{u}}} \propto \frac{1}{\sqrt{Sc}} \qquad Sc \equiv \frac{\nu}{D} \quad \text{(Schmidt number)}$$

- Boundary layer thickness at the moving interface
  - Velocity field: $\delta_{\mathrm{u}} \propto L / \sqrt{Re}$
  - Concentration field: $\delta_{\mathrm{c}} \propto L / \sqrt{Pe} = L / \sqrt{ScRe}$

$$\frac{\delta_{\mathrm{c}}}{\delta_{\mathrm{u}}} \propto \frac{1}{\sqrt{Sc}}$$

Disparity of length scales (cont.)

- Typical values of the Schmidt number
  - Gases $Sc = O(1)$
  - Liquids $Sc = O(1000)$

$$\frac{\lambda_c}{\lambda_u} \approx \frac{\delta_c}{\delta_u} \approx \frac{1}{\sqrt{1000}} = \frac{1}{31.6}$$

- The smallest length scales in the concentration field are about a factor of 30 smaller than those in the velocity field
- The grid required for resolving all scales in the concentration field is 30 times finer than required for the velocity field (in 3D this corresponds to a factor of 30^3 = 27 000)
- This makes numerical methods that use the same grid for the velocity and concentration field very inefficient
  $\Rightarrow$ use of hierarchical grids, i.e. a finer grid for the concentration field than for the velocity field (ongoing PhD)

Conclusions

- High potential of Taylor flow for intensification of heterogeneously catalyzed gas-liquid processes in micro reactors
- Complicate interaction between two-phase flow, transport (heat and mass) and 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
- Current status of numerical methods
  - 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 detailed chemical kinetics*

Outlook

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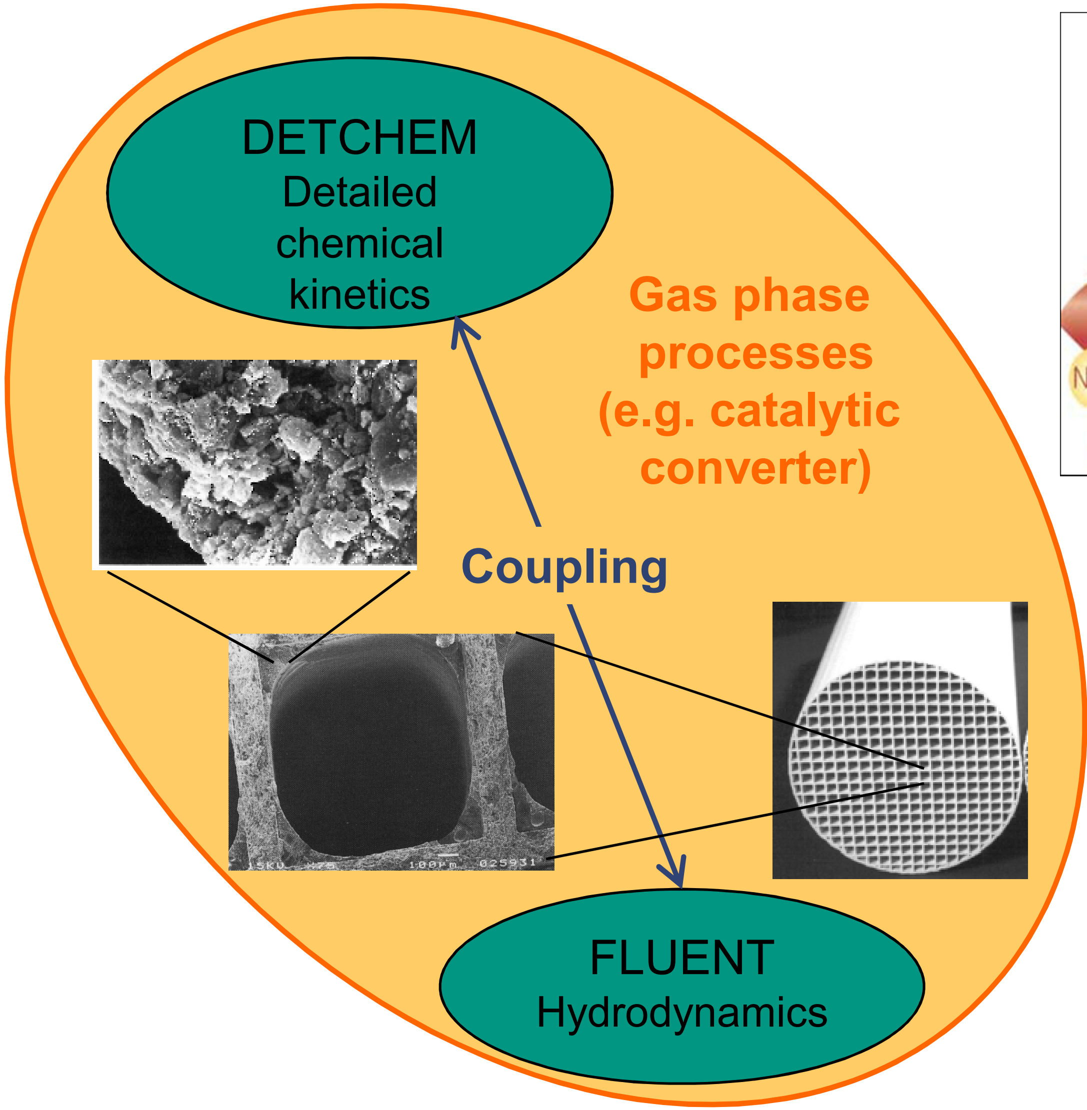
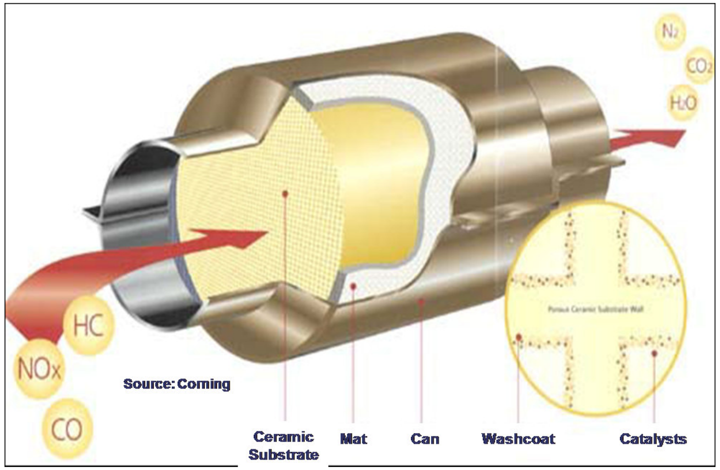




Outlook

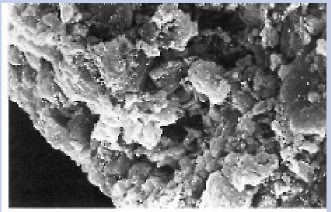
Kinetics for FTS

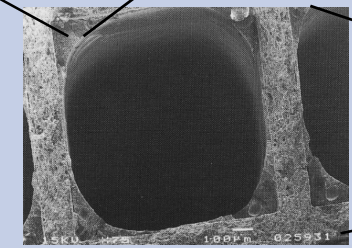
DETCHEM
Detailed chemical kinetics at channel walls

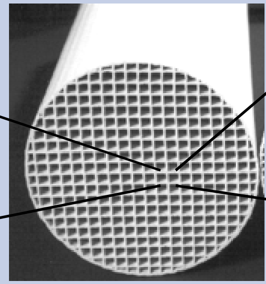
Coupling

TURBIT-VOF
Detailed simulation of two-phase flow and transport within channel

Two-phase processes in monolith reactors (e.g. Fischer-Tropsch synthesis)







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  - Murat Öztaskin
  - Semih Kececi
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