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Numerical Simulation of Interfacial Mass Transfer Accompanied by a First-Order Chemical Reaction in Segmented Gas-Liquid Flow within a Mini-Channel

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Introduction

Advantages and applications of segmented gas-liquid flow in square narrow channels:

- Monolithic catalyst reactor: gas bubbles segment the liquid and enhance its mixing
- Micro bubble column: efficient mass transfer due to high interfacial area per unit volume
- Goal: Get insight in local instantaneous mass transfer phenomena by means of direct numerical simulations

Numerical method

- In-house code TURBIT-VOF solves incompressible Navier-Stokes equation with surface tension by a Volume-of-Fluid method with local planar interface reconstruction
- Implementation of species transport equation under assumption of no feed-back on hydrodynamics
- The physical concentration field c is transformed into $\tilde{c}$ which is continuous at the interface

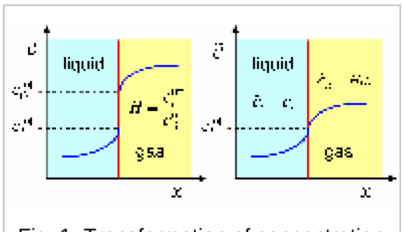

Fig. 1: Transformation of concentration field c into $\tilde{c}$ using Henry number H.

Bubble train flow

Hydrodynamics

- Developed bubble train flow (BTF) is fully described by a unit cell (UC) with one bubble and one liquid slug
- BTF is numerically represented by one unit cell and periodic boundary conditions in vertical axial direction (see Fig. 2)

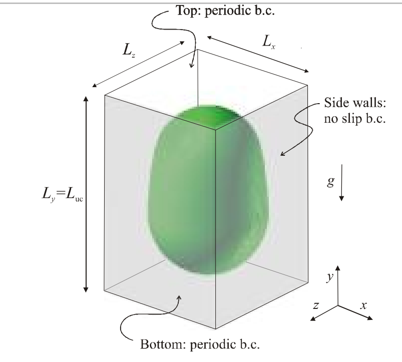

Fig. 2: Sketch of computational domain.

- Simulations of air / silicon oil BTF in a square channel with $L_x = L_z$ = 2 mm for three different unit cell length L_{uc} = 2, 2.75 and 3.5 mm and a void fraction e = 33%
- Computed bubble diameter and velocity are in good agreement with experimental data [1]

Mass transfer

- Mass transfer of an artificial species from gas phase (initial concentration c_G^0) into the liquid phase (initial concentration 0)
- Simulations for mass transfer with and without 1st order homogenous (liquid bulk) and heterogeneous (channel walls) chemical reaction
- Henry number $H \equiv (c_L\ /\ c_G)_{eq.}$ = 0.03 and 3, D_L/D_G = 0.31; liquid phase Schmidt number = 0.8; bubble Reynolds number = 10

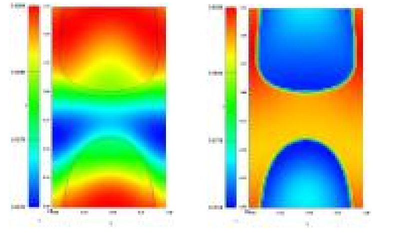

Fig. 3: Concentration field $\tilde{c}$ for H = 0.03 (left) and c for H = 3 (right) in vertical mid-plane for $t \approx$ 0.01s.

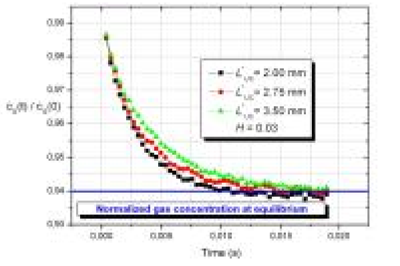

Fig. 4: Mean concentration $c_G(t)$ for H = 0.03 and different values of L_{uc}. For small L_{uc} the equilibrium concentration $c_G^{eq} = c_G^0/(1+H(1/e-1))$ is reached faster.

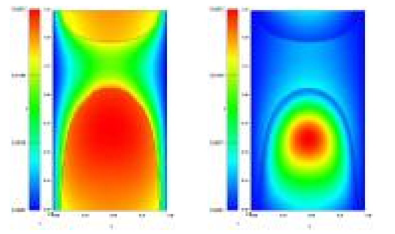

Fig. 5: Concentration field $\tilde{c}$ for H = 0.03 (left) and H = 3 (right) in a vertical mid-plane for mass transfer with heterogeneous chemical reaction.

Conclusions

- Mass transfer occurs mainly across the bubble tip and bottom (in agreement with [3]), while the liquid film is saturated (Fig. 3)
- Short unit cells are more efficient for mass transfer with / without homog. chemical reaction (Fig. 4)
- Long unit cells are slightly more efficient for mass transfer with heterogeneous chemical reaction in case of small Henry number and fast film saturation

Literature:

[1] Thulasidas, Abraham, Cerro: *Chem. Eng. Sci.* **50** (1995) 183-199
[2] Ghidersa, Wörner, Cacuci: *Chem. Eng. J.* **101** (2004) 285-294
[3] Berčič & Pintar: *Chem. Eng. Sci.* **52** (1997) 3709-3719

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