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Mass transfer and catalytic reaction in Taylor flow: parametric numerical study for frozen hydrodynamics

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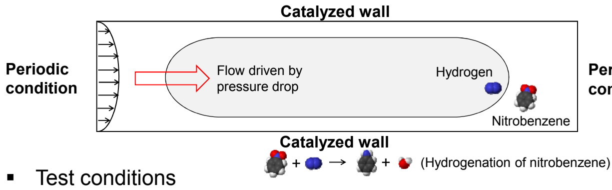
Objectives

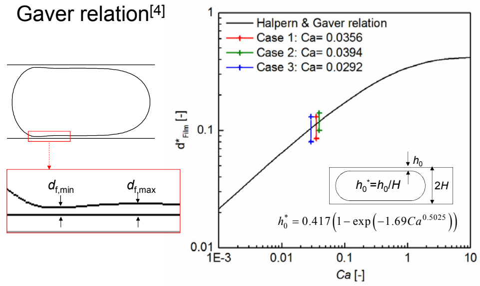
- Goal: Simulation of catalyzed hydrogenation of nitrobenzene to aniline within a Taylor flow in monolith reactor
- Methodology
  - Coupling two computer codes: TURBIT-VOF[1] for the gas-liquid flows and DETCHEM[2] for the reaction kinetics
  - Moving reference frame approach for mass transfer
  - Langmuir-Hinshelwood type global reaction kinetics[3]



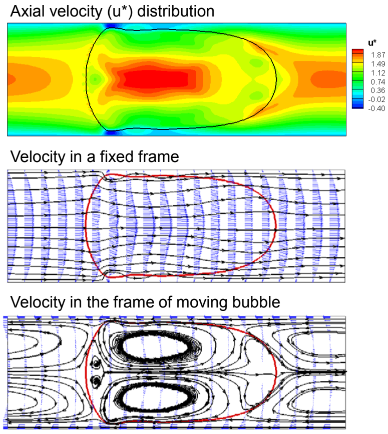
- Test conditions
  - Temperature: 298K, pressure: 7bar, channel height: 100µm
  - Reynolds number: 80~110, capillary number: 0.03~0.04

Numerical approaches

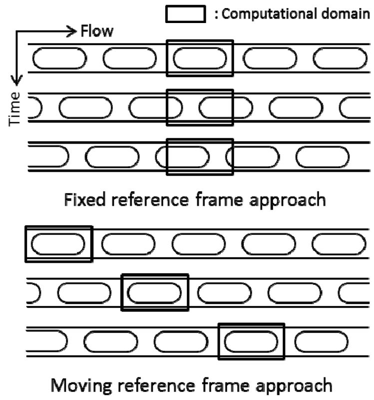
- Hydrodynamics
  - Two-dimensional incompressible Navier-Stokes equation with Volume-of-fluid (VOF) method
  - Isothermal simulation
  - Constant physical properties during calculation
  - Fine mesh resolution near the boundary wall
  - Comparison of film thickness with Halpern & Gaver relation[4]



- Velocity fields for different Reynolds and capillary number (case 1)

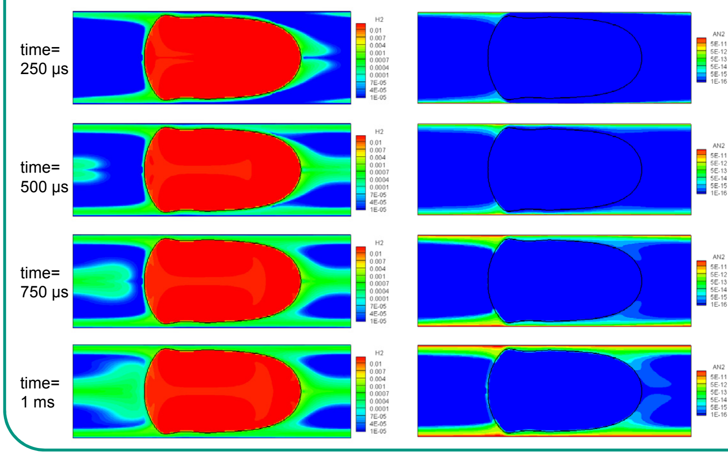


- Mass transfer in the moving frame
  - Solve concentration equations with frozen hydrodynamics at quasi steady state

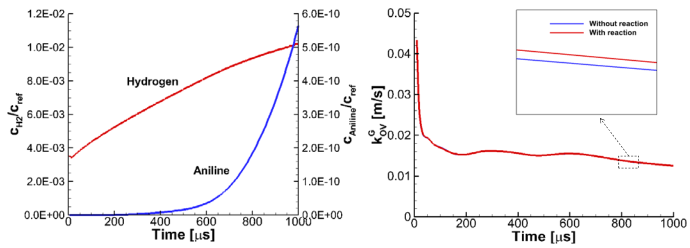


Results of reactive mass transfer in the moving frame

- Temporal distributions of hydrogen and aniline



- Mean concentrations and mass transfer coefficient



- Hydrogen mass transfer is largest at the rear part of the bubble where the liquid film thickness is thinnest
- The aniline is mainly produced in rear part as well
- The mean concentration of hydrogen in liquid phase is increasing by mass transfer from the gas phase and that of aniline is also increasing due to the reaction
- The enhancement of mass transfer coefficient by reaction is small

Conclusions

- The gas-liquid Taylor flow of nitrobenzene and hydrogen has been successfully computed with real viscosities and diffusivities
- Moving frame approach allows to save the computational time without loss of physical information
- The estimation of film region is most important to investigate the catalytic reaction within the Taylor flow

References

[1] Onea et al., Chem. Eng. Sci., 64 (2009) 1416-1435

[2] Deutschmann et al, DETCHEM™ User Manual, 2012, http://www.detchem.com

[3] Höller et al., Chem. Eng. Technol. 23 (2000) 3, 251-255

[4] Halpern et al., J Comput Phys, 115(2) (1994) 366-375

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