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A Numerical Study on Gas-Liquid Taylor Flow for Catalytic Hydrogenation of Nitrobenzene with Detailed Kinetic Mechanism

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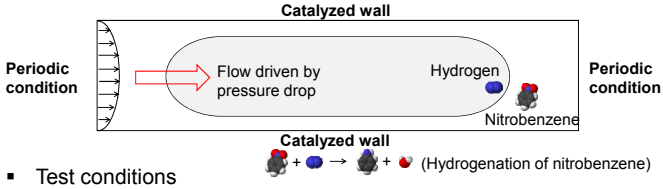
Objectives

- Simulation of the heterogeneously catalyzed hydrogenation of nitrobenzene to aniline for Taylor flow in a monolith reactor
- Methodology
  - Coupling two computer codes: TURBIT-VOF [1] for the gas-liquid flow and DETCHEM™ [2] for the reaction kinetics at the wall
  - Moving reference frame approach for mass transfer simulations
  - Detailed reaction mechanism based on density functional theory

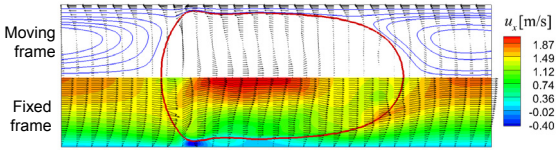


- Test conditions
  - Temperature T = 323 K, pressure p = 7 bar, channel height h = 100 µm
  - Reynolds number $Re=\rho_L h U_B/\mu_L=120$, capillary number $Ca=U_B\mu_L/\sigma=0.044$

Numerical approaches

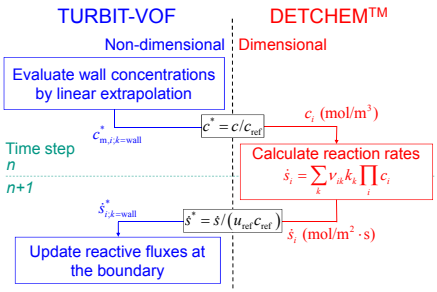
Hydrodynamics

- Two-dimensional incompressible Navier-Stokes equation with Volume-of-fluid (VOF) method
- Isothermal simulation, no phase change
- Constant physical properties
- Simulation in fixed frame of reference till quasi-steady state



Quasi-steady state velocity field of the Taylor flow in fixed (bottom half) and moving (upper half) frame of reference

Coupling of the two codes

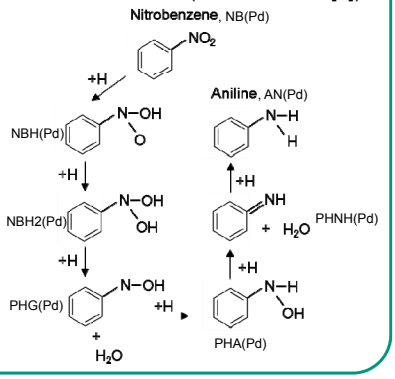


Mass transfer in moving reference frame

- Concentration equations are solved with frozen velocity field from hydrodynamic simulation
- One way coupling, no homogeneous reaction

Reaction mechanism

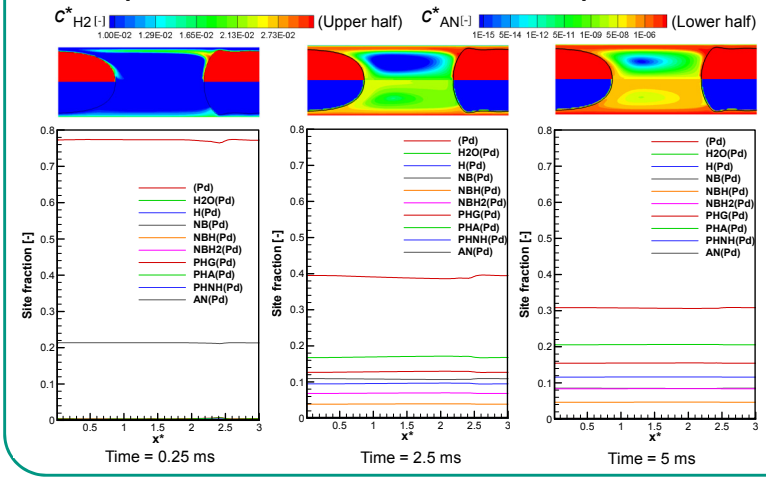
- 3 bulk species, 10 surface species
- Reaction path from nitrobenzene to aniline for T>400 K (mechanism B [3])*



* Reaction rate at 1500 K is utilized for qualitative analysis

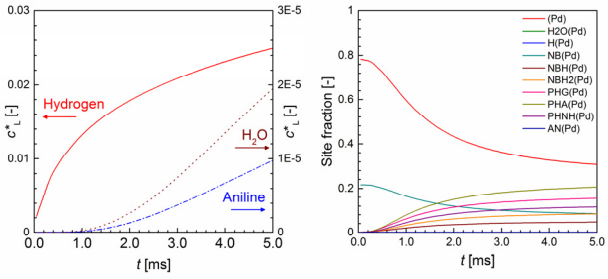
Reactive mass transfer with a Taylor flow

Temporal distributions of bulk and surface species



Time = 0.25 ms | Time = 2.5 ms | Time = 5 ms

Time evolution of bulk and surface species



- Hydrogen mass transfer is largest at the rear part of the bubble where the thickness of the liquid film is thinnest
- Aniline is mainly produced in the rear part of the liq. film as well
- An axial variation of surface species appears at the beginning of the mass transfer simulations and then gradually diminishes
- Hydrogen is transferred from the bubble while H_2O and aniline are produced by reaction as well as change of surface species

Conclusions

- Development of computer code for gas-liquid Taylor flow with surface reaction has been accomplished by coupling TURBIT-VOF/DETCHEM™
- Moving reference frame approach allows saving computational time supposed the feedback of mass transfer on hydrodynamics is negligible
- Using a detailed reaction mechanism, a qualitative analysis on the coupling between bulk and surface species has been accomplished

References
[1] A. Onea et al., Chem. Eng. Sci. **64** (2009) 1416-1435
[2] O. Deutschmann et al., DETCHEM™ User Manual, 2012, http://www.detchem.com
[3] L. Zhang et al., RSC. Adv. **5** (2015) 34319

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