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PROCESSNET
P56

Development of a Computer Code for Numerical Simulation of Reactive and Catalytic Two-Phase Flows with Detailed Chemistry

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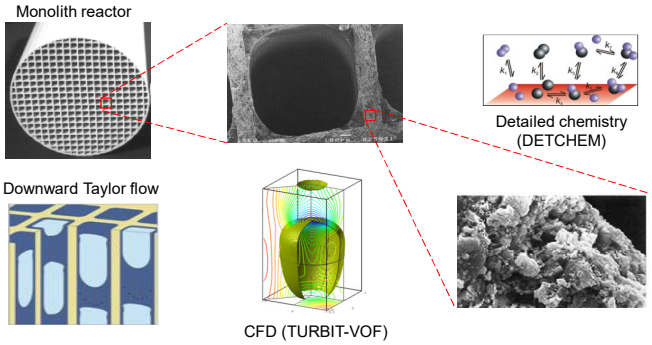
Objectives

- The development of a computer code for detailed numerical simulations of heterogeneously catalyzed reactions in gas-liquid flows in a single channel of a monolith reactor
- Coupling two in-house computer codes
  - TURBIT-VOF for the gas-liquid flows
  - DETCHEM for the reaction kinetics
- Here: Verification and validation of the coupled solver for diffusion-reaction problems



Diffusion models

Multicomponent model

- Consider diffusivity matrix among all species
- High accuracy and high computational cost

$$\mathbf{j} = -\mathbb{B}^{-1} \cdot \frac{\partial \mathbf{c}}{\partial z} \qquad \mathbf{j} = \left(j_1, j_2, \cdots, j_n\right)^T, \ \mathbf{c} = \left(c_1, c_2, \cdots, c_n\right)^T$$

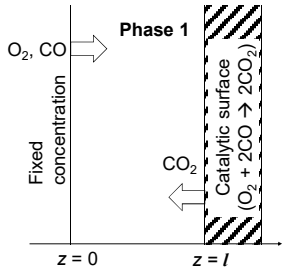
$$B_{ii} = \frac{c_i}{D_{in}} + \sum_{\substack{k=1 \\ i \neq k}}^{n} \frac{c_k}{D_{ik}}, \quad B_{ij} = -c_i \left(\frac{1}{D_{ij}} - \frac{1}{D_{in}} \right)$$

Effective diffusivity model (Mixture-averaged diffusion model)

- Assume the species i diffuses through the mixture of the rest (n-1) of species
- Low computational cost, reasonable accuracy

$$j_i = -D_{i,\text{eff}} \frac{\partial c_i}{\partial z} \qquad D_{i,\text{eff}} = \left(1 - c_i\right) / \left(\sum_{\substack{j=1 \\ j \neq i}}^{n} \frac{c_j}{D_{ij}} \right)$$

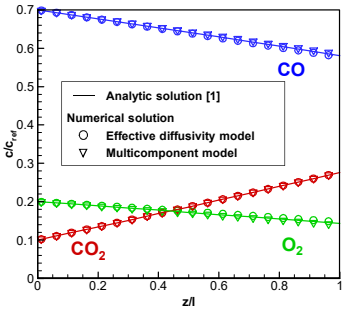
Validation 1



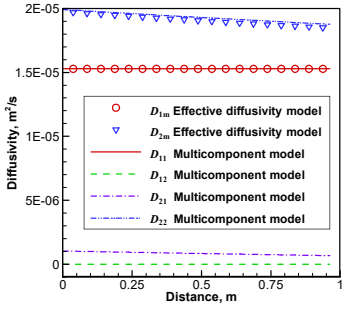
Multispecies in single phase

- CO-oxidation at the catalytic surface in gaseous phase
- Assumption for diffusivity (for analytic solution)

$$D_{CO\text{-}CO_2} = D_{O_2\text{-}CO_2}$$

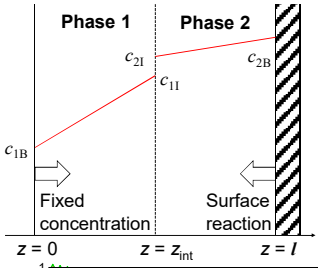


Concentration profiles computed by different diffusion models



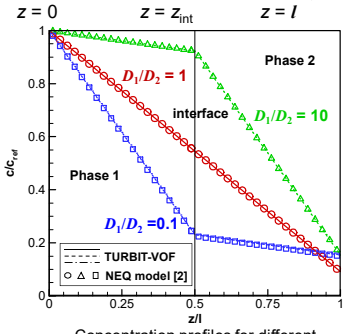
Comparison of the diffusivities for different diffusion models

Validation 2

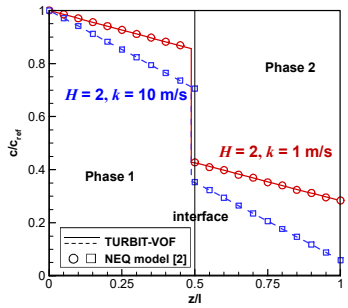


Multiphase with various parameters

- Diffusion-reaction studies with respect to
  - Diffusivity ratio
  - Henry number
  - Reaction rate



Concentration profiles for different diffusivity ratios (H = 1, k = 10 m/s)



Concentration profiles with respect to reaction constants

Conclusions and outlook

- The multispecies diffusion with heterogeneous reaction has been validated for single phase and two-phase with planar interface
- The effective diffusivity model can be used for further investigations, since it is sufficiently accurate with less computational effort
- In the next step, mass transfer with the sample surface reaction of the Energy Alliance (Hydrogenation of Nitrobenzene to Aniline) will be studied in the two phase flow with planar interface and in Taylor flow

References

[1] R.B. Bird, W.E. Stewart, E.N. Lightfoot, Transport Phenomena 2nd ed., J. Wiley & Sons, New York, 2002, ISBN 0-471-41077-2

[2] E. Kenig, A. Gorak, A film model based approach for simulation of multicomponent reactive separation, Chemical Engineering and Processing, 1995, 34, 97-103