Catalytic Pellet Based
Heterocatalytic Reactor Bed Models Development

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The aim of the work

- Two-phase model development
- Micro level investigation
- Catalytic pellet model – bed model
Modelling with CFD technics

• COMSOL Multiphysics 3.5a:
  – Solve PDE with Finite element method
  – Complex modelling surface
  – User friendly implementation
  – Many fields specialised toolbox

• MATLAB:
  – Numbers of functions
  – Communication with COMSOL Multiphysics
  – High performance of visualistion tools
The studied object

- **Reaction**
  \[ A + B \rightleftharpoons C \]

- **The properties of the reaction:**
  - Equilibrium reaction
  - Exothermic
  - Number of moles is changing

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The implementation of the models

Temperature [K]

Concentration, cA [mol/m³]

Experiment

Calculate
Motivations of this presentation

• To show the method of investigation the heterocatalytic phenomena on micro level

• To show a new modelling concept:
  – To build complex network from simple models
Results

Concentration of raw material

Concentration of product

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Results

Temperature

Velocity

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The models of catalytic bed

Examined model

Reference model
Calculation of the difference

\[
\frac{(\text{Ref.profile} - \text{Result.profile})^2}{(\text{Max.value} - \text{Min.value})^2}
\]

vectors

 scalars
Difference between the velocity profiles

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Difference between the concentration of raw material (A,B) profiles

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Difference between the concentration of the product (C) profile
Aggregated results

Particle size dependence of the aggregated relative squared difference of the reference and the built catalyst bed parameters

- cA
- cB
- cC
- v
- T_sec_axis

Aggregated relative squared difference vs. Pellet diameter (mm)
Conclusion

• Two dimensional model of a catalyst pellet with its close surroundings was implemented

• Catalytic beds was implemented pellet by pellet with the network modelling concept and the validation of results has been started

  – **Advantages:**
    • Reduced memory needs
    • You can work with a simple PC

  – **Disadvantages:**
    • Slow
    • Inaccurate
    • It works with only special models
Plans for model improvement in the future

- Automation of the bed builder
- Work with pellet structures as an element
- Expansion the domains of the parameters:
  - Pellet diameter
  - Work in 3 space-dimension
- Identification of the back-mixing effect with iterative methods

- With the advanced model:
  - Optimization of catalytic pellet:
    - geometry
    - shape
    - distribution in the catalytic bed
  - Analyze the operation of reactor
  - Sensitivity examination
Thank you for your attention!

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C'est la fin