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Catalytic Pellet Based Heterocatalytic Reactor Bed Models Development

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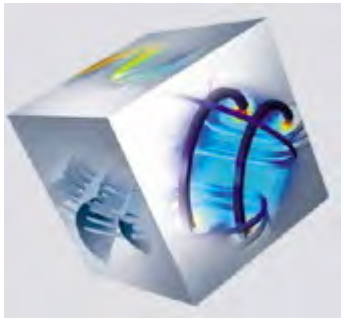
The aim of the work

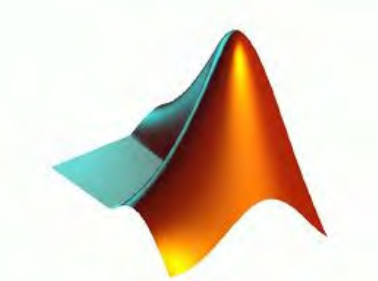
- **Two-phase model development**
- **Micro level investigation**
- **Catalytic pellet model – bed model**

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

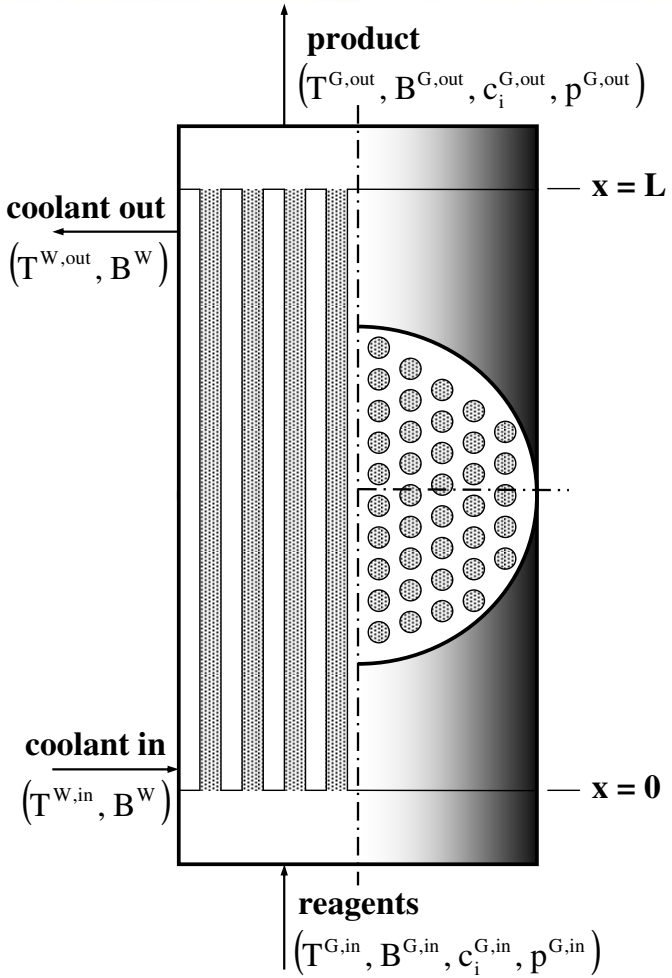


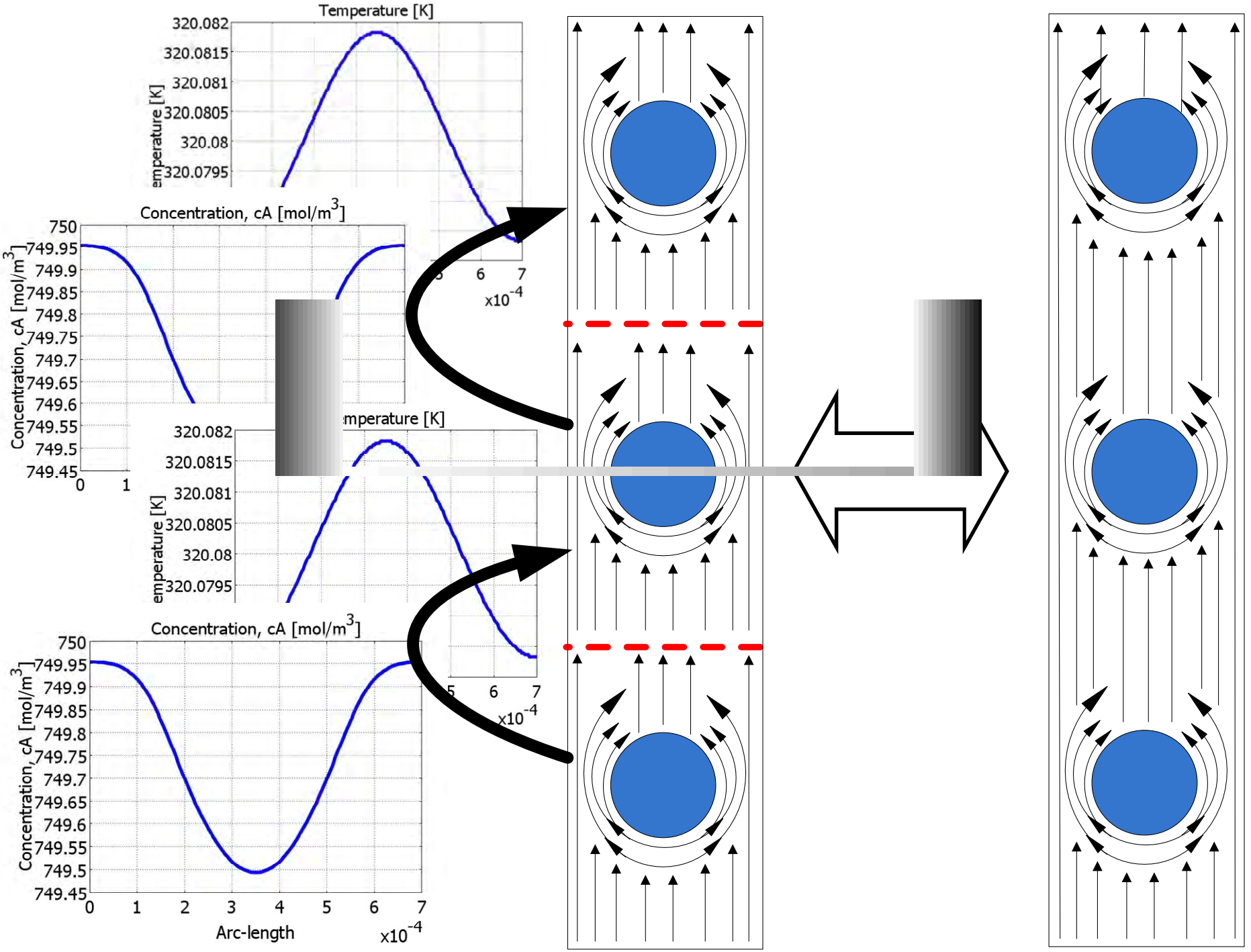
The studied object

- **Reaction**

$$A + B \Leftrightarrow C$$

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



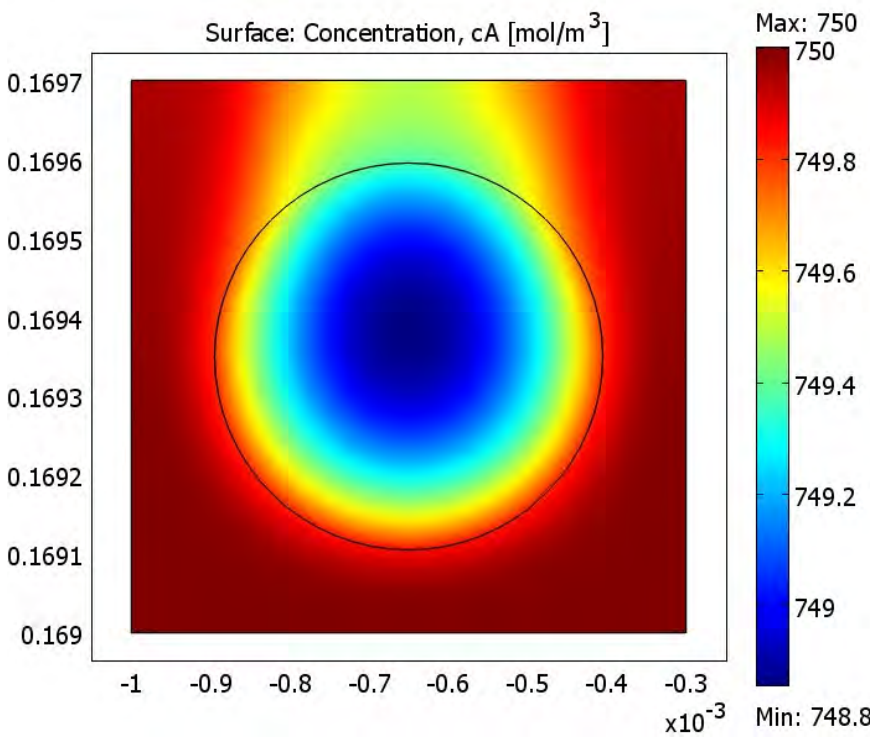

Temperature [K]
320.082
320.0815
320.081
320.0805
320.08
320.0795
emperature [K]
Concentration, cA [mol/m3]
750
749.95
749.9
749.85
749.8
749.75
749.7
749.65
749.6
749.55
749.5
749.45
Concentration, cA [mol/m3]
0
1
2
3
4
5
6
7
x10-4
Arc-length

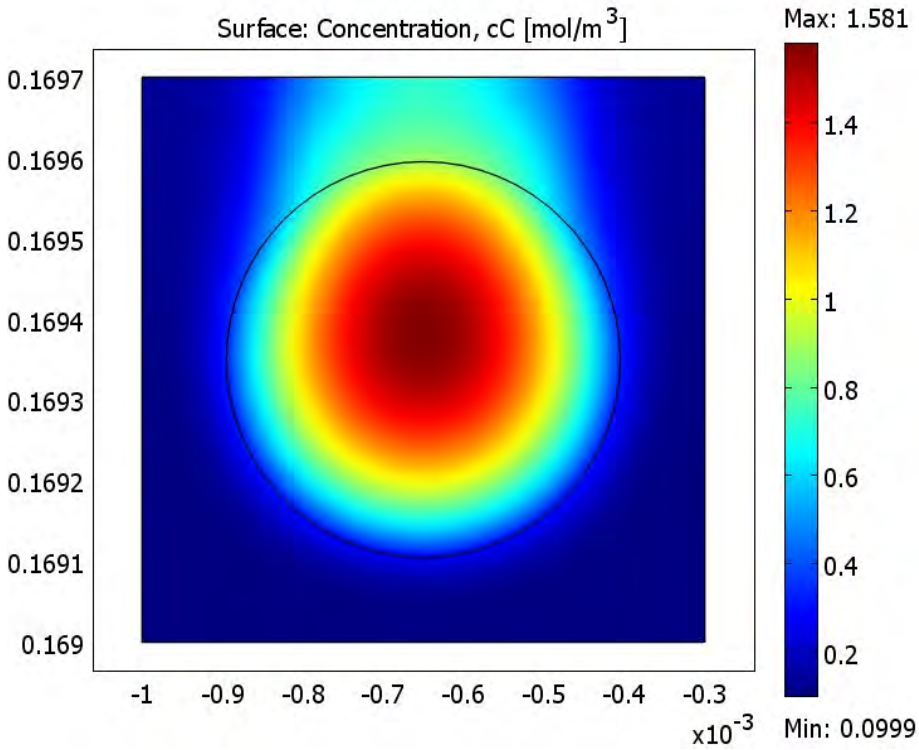
Motivations of this presentation

- **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

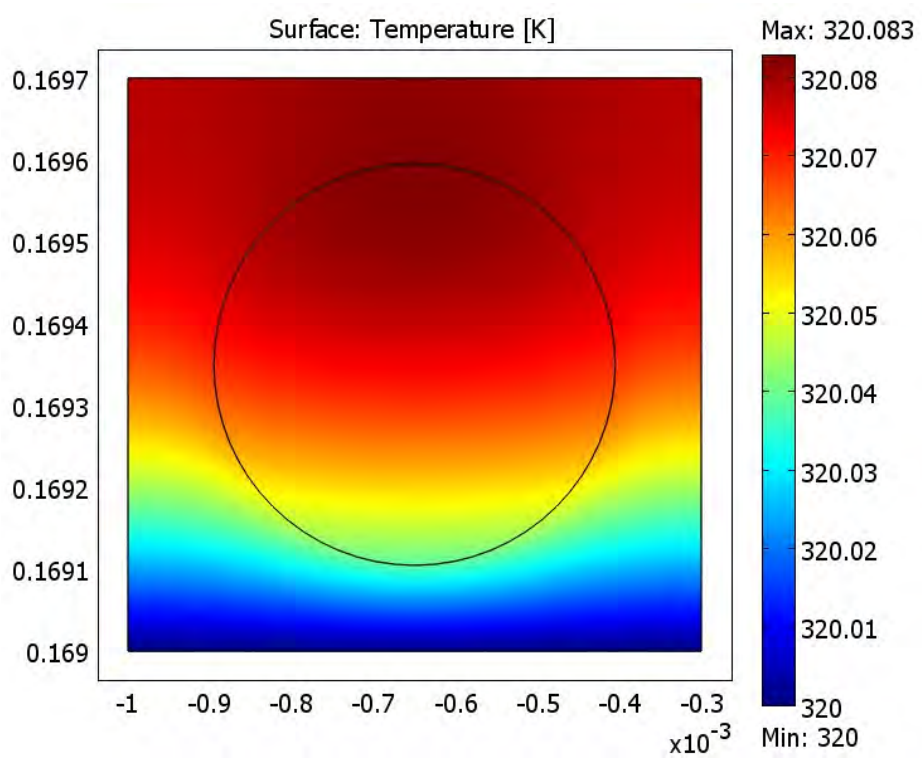




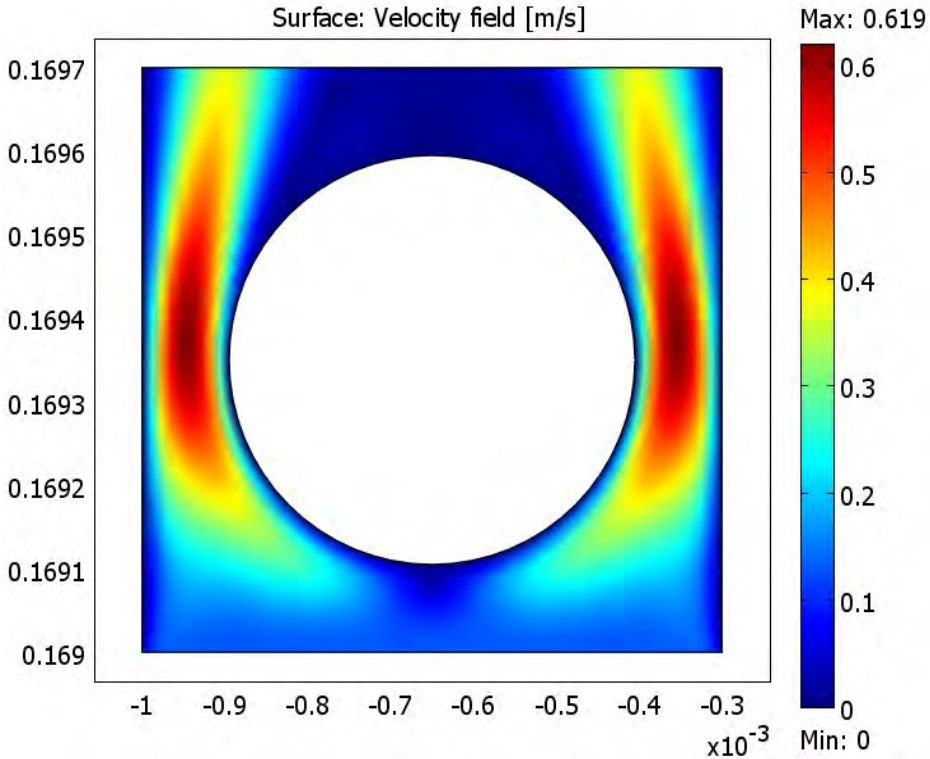
Concentration of raw material

Concentration of product

Results



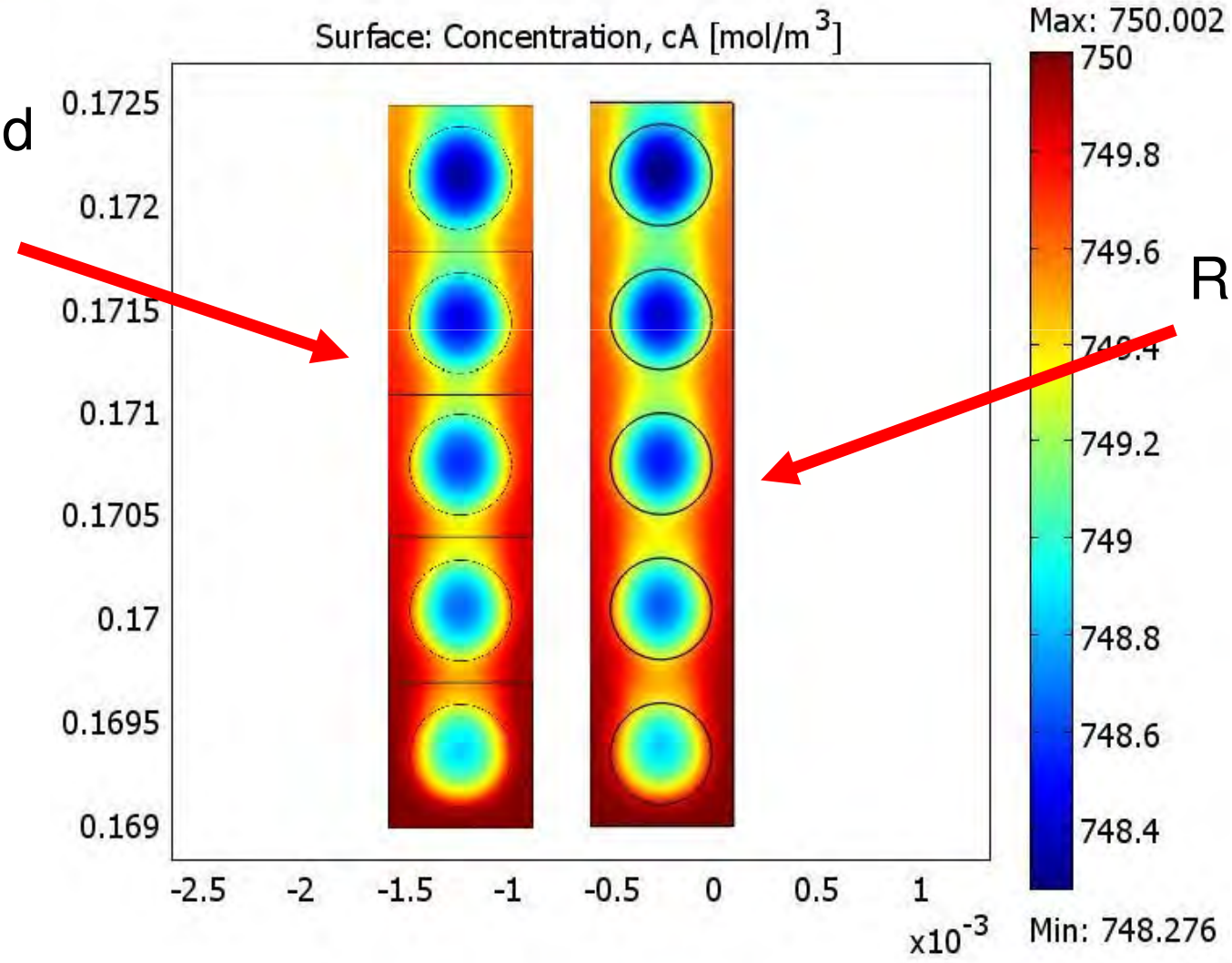
Temperature



Velocity

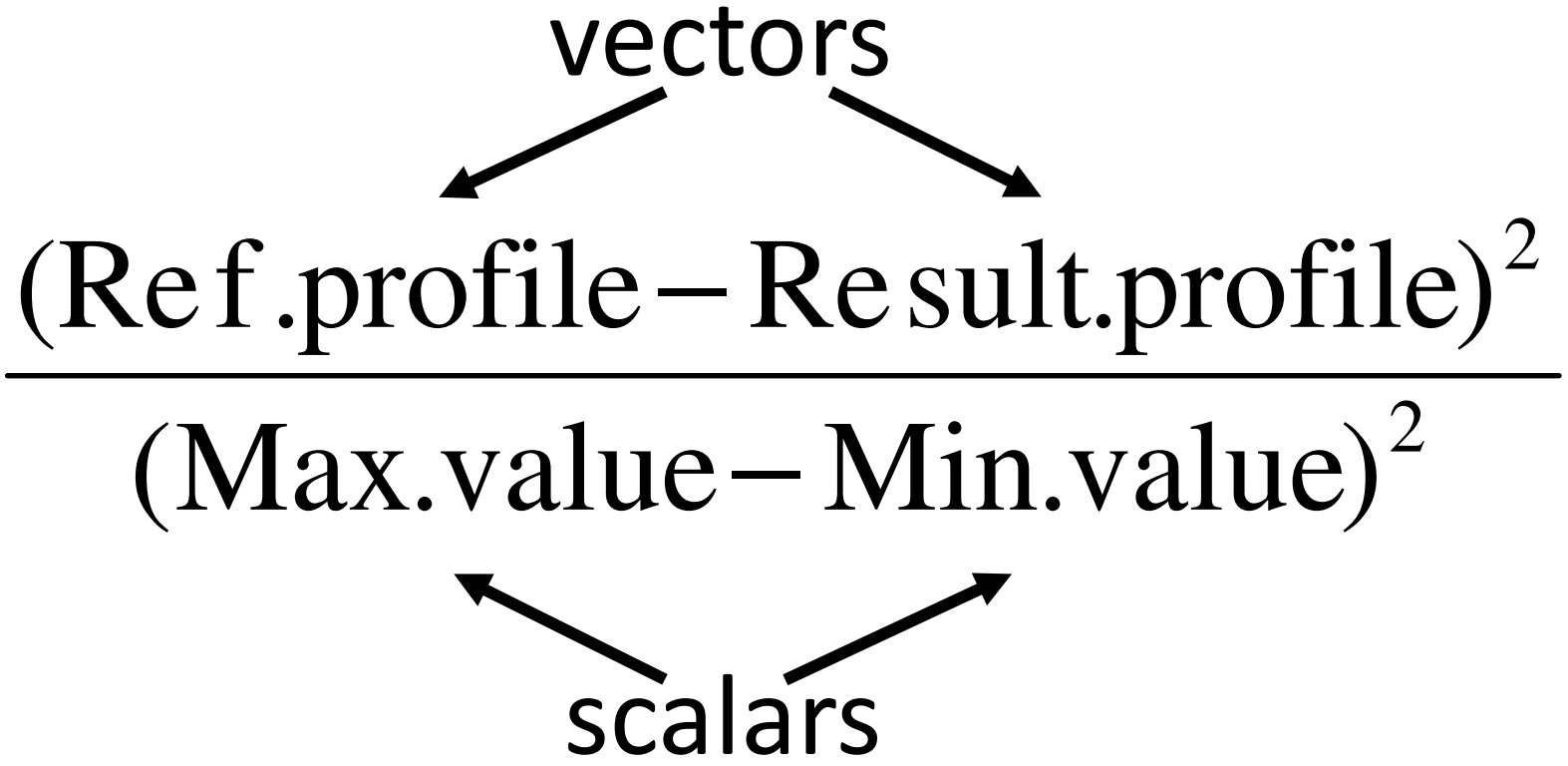
The models of catalytic bed

Examined model

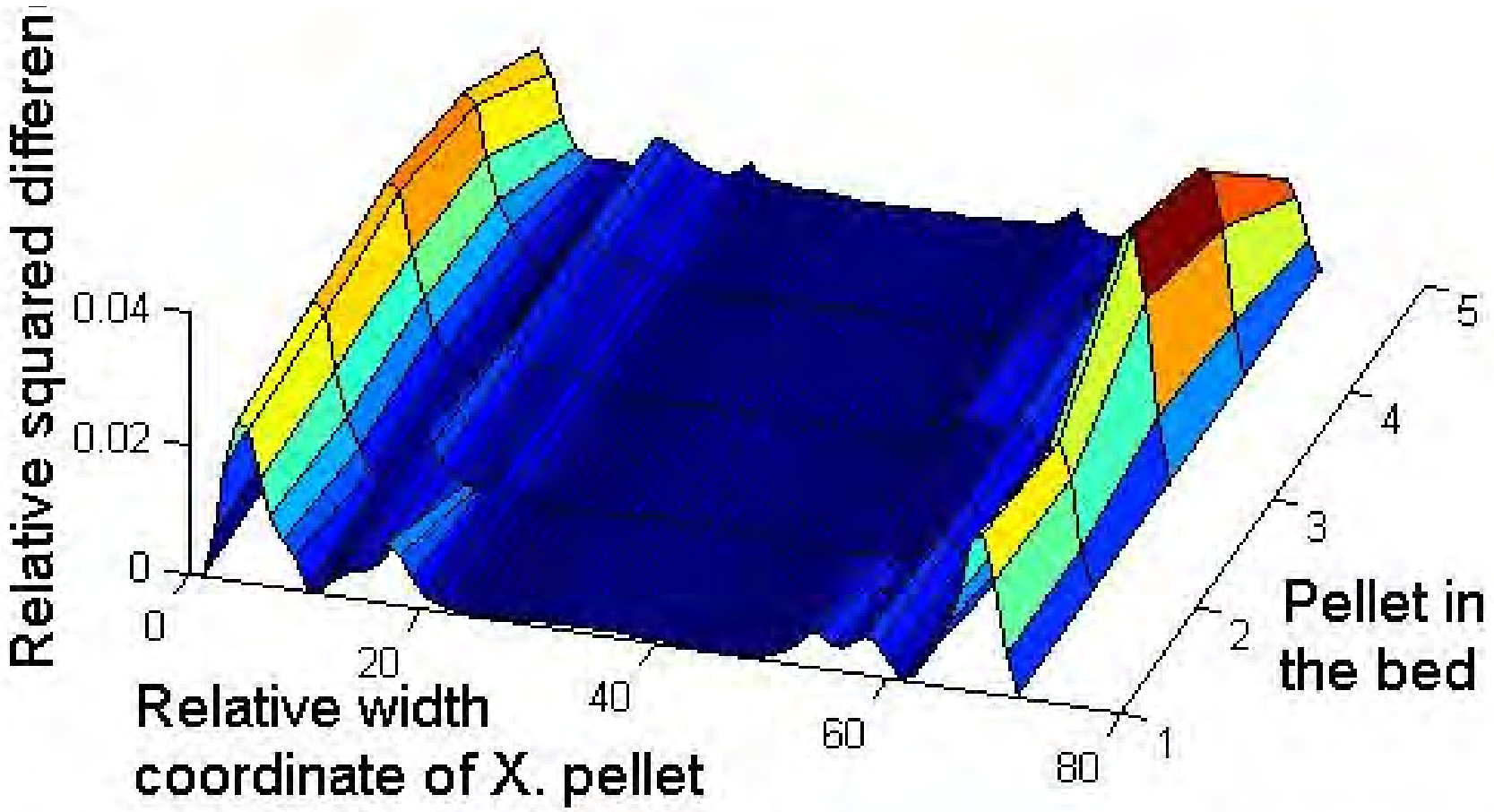


Reference model

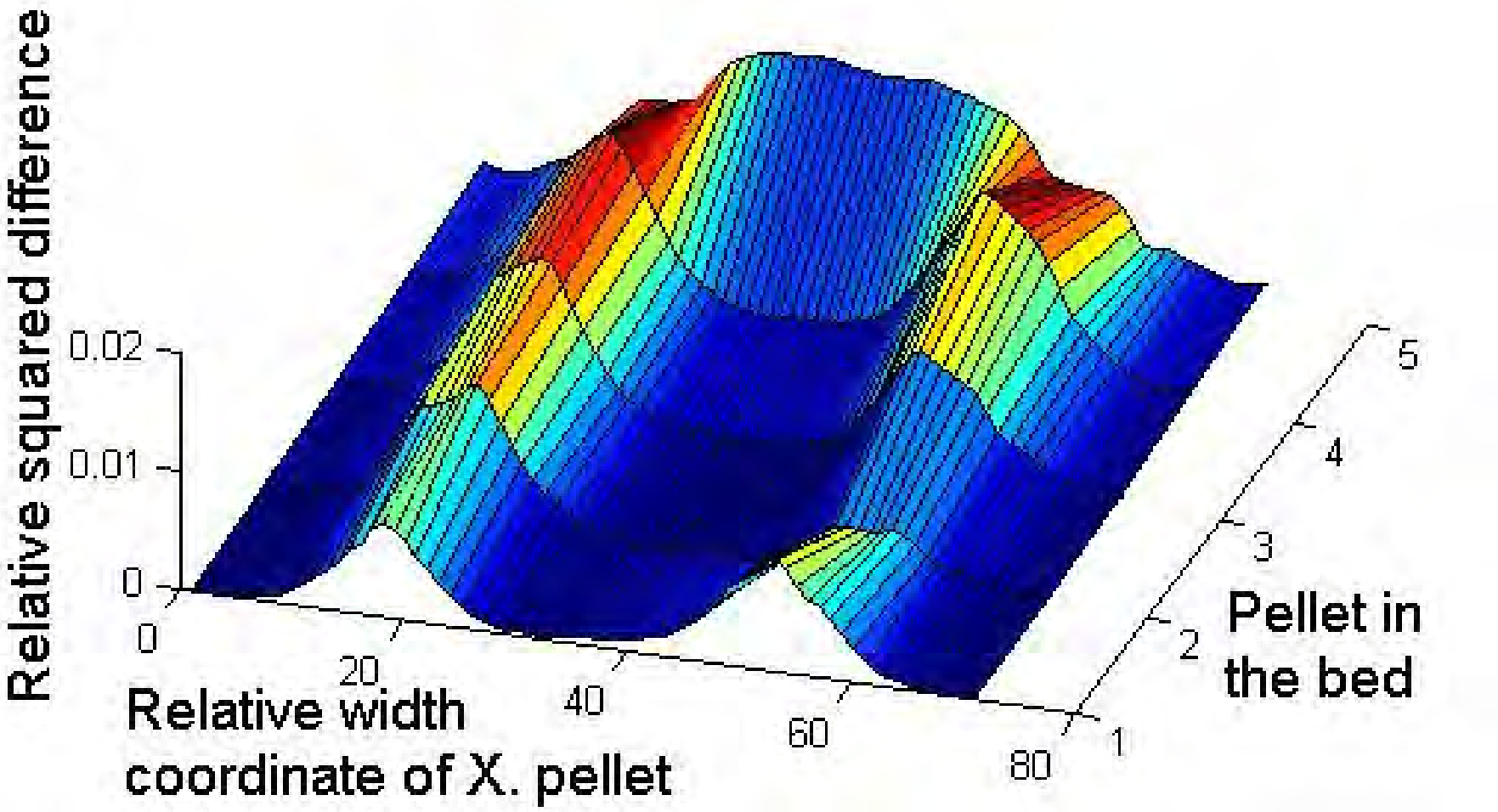
Calculation of the difference



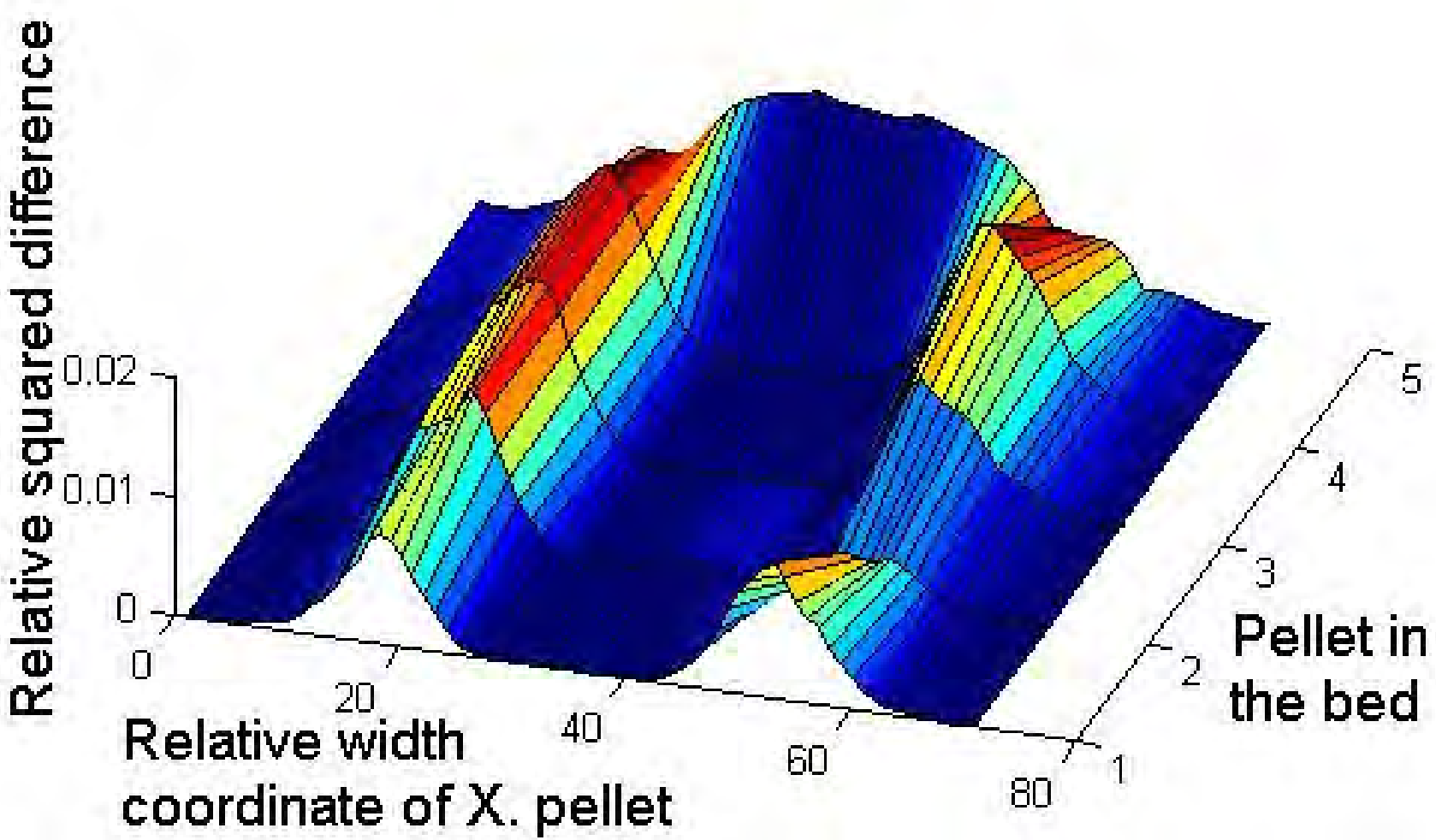
Difference between the velocity profiles



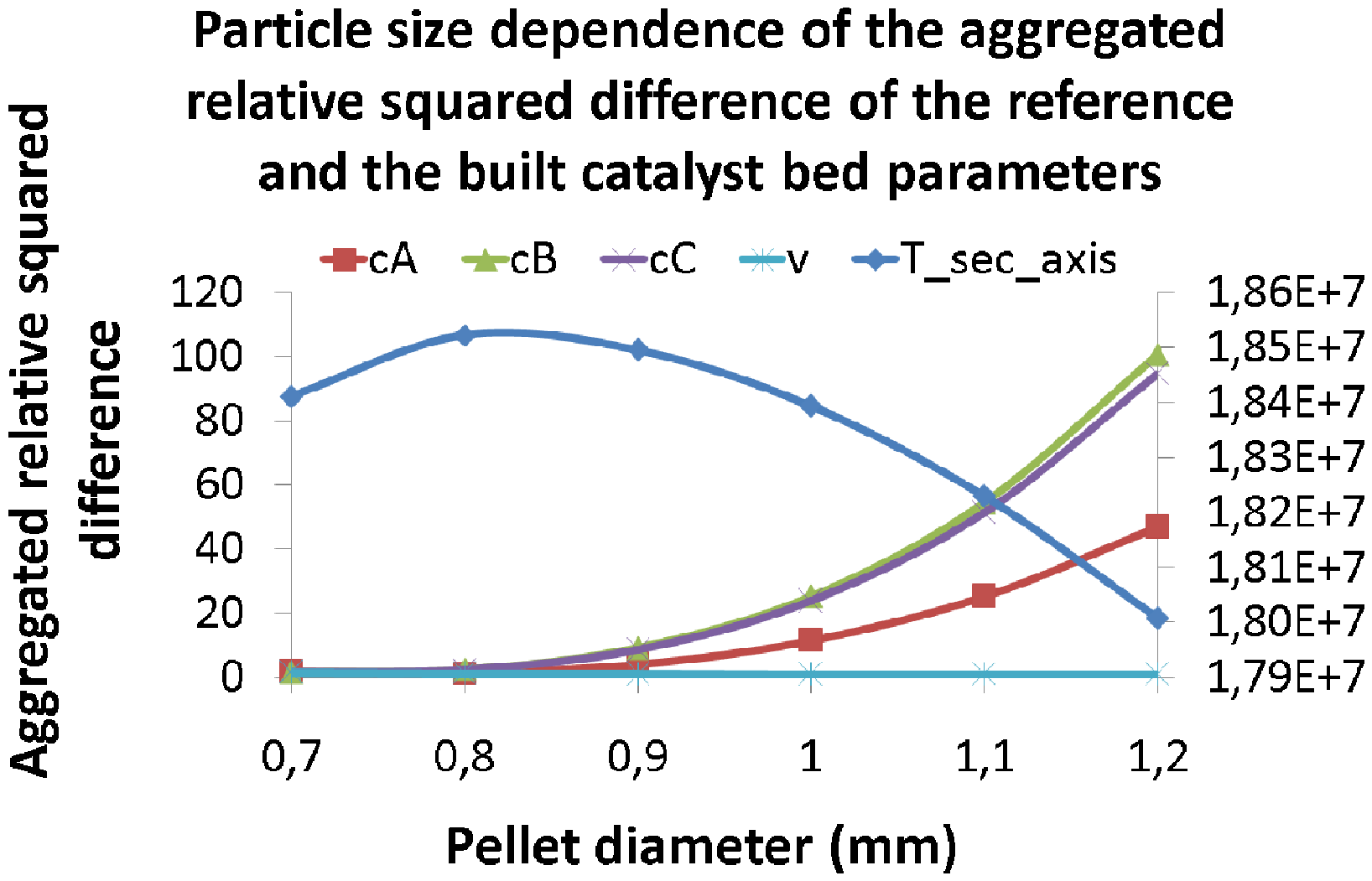
Difference between the concentration of raw material (A,B) profiles



Difference between the concentration of the product (C) profile



Aggregated results



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!

Acknowledgements:

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