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Master Thesis Topic

Numerical investigation of core-shell catalyst pellets and their influence on the performance of fixed-bed reactors

The Max Planck Institute for Dynamics of Complex Technical Systems is looking for a student (m/f/d) for a Master's thesis within the Process Systems Engineering Group starting as of now. The thesis deals with the numerical investigation of catalyst pellet design on the performance of fixed-bed reactors, which are a key technology for large scale low cost chemical synthesis. Further information about the topic can be found at https://doi.org/10.1016/j.cej.2019.123704.

Motivation

In the chemical industry, the production of a wide range of products takes place as heterogeneously catalyzed gas-phase reaction in catalytic fixed-bed reactors. Especially multi-tubular reactors are frequently used for reactions with strong exothermicity, since the high surface-to-volume ratio favors energy transfer via the reactor wall. The efficiency of such reactors can be increased by various methods of process intensification. With regard to heat management, dilution of the catalytic fixed-bed bed by addition of inert material is a well-established method. Often the reactor has different zones in axial direction, which are characterized by different degrees of dilution, in order to adjust the local energy release as well as the local heat transport. The goal of these methods is to set an optimal reaction temperature while maintaining system-specific constraints.
In this context, our research has shown that the use of core-shell catalyst pellets, consisting of a catalytically active core, which is surrounded by an inactive, but porous shell, is favorable for some cases. A detailed comparison to fixed-bed dilution with inert catalyst pellets has revealed that the benefits arise from the mitigation of the reaction rate by the inert shell in particular at high reactor temperatures. Hence, the inert shell prevents significant temperature excursions, which could damage catalyst and reactor material, while allowing for high reactant conversions at the same time. Especially the occurrence of so-called thermal runaways can be avoided in this way. However, the inert shell has also been shown to affect the selectivity of the reaction system. The reason for this is a non-intuitive interaction of the chemical equilibria and mass transfer rates in the catalyst pellets.

Aim of this thesis

The task of the thesis is the numerical investigation of core-shell catalyst pellets with regard to their influence on the selectivity of a fixed-bed reactor. For this purpose, an existing Matlab code is adapted. By employing sensitivity analyses,

suited optimization variables are chosen for subsequent optimization studies. Based on the results of the optimization, a qualitative statement if and when the product yield (or selectivity) of the reactor is improved by core-shell catalyst pellets is derived. The results are interpreted, critically analyzed and presented in written form in a clear and descriptive manner.

Work packages

- Familiarization and extension of an existing Matlab code
- Carrying out sensitivity analyses and numerical optimization studies to identify the applicability of core-shell catalyst pellets to partial oxidation reactions
- Derivation of principles, when core-shell catalyst pellets appear to be promising for systems with selectivity issues

Requirements

- Completed Bachelor's degree in chemical engineering, biosystems engineering, environmental and energy process engineering, or similar technical degree program
- Experience with programming software, preferably in Matlab
- Knowledge and interest in mathematical modelling, simulation and optimization

Start: according to arrangement
Working mode: home office / in presence at MPI (Sandtorstraße 1, 39106 Magdeburg)
Language: German or English

Supervisor: Ronny T. Zimmermann, M. Sc.
1st Reviewer: Prof. Dr.-Ing. Kai Sundmacher
2nd Reviewer: t.b.d.

If interested, please contact us with your curriculum vitae and an overview of grades at:

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