Reactor Optimization by a Model-Based Approach for Heterogeneously Catalyzed Endothermal Reactions

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Introduction

In the chemical process industries the implementation of energy-efficient processes with reduced carbon dioxide emissions has become one of the top priorities. Therefore, intensification and optimization of existing processes, especially of chemical reactors, is crucial for achieving these goals and enhancing productivity. In this regard, an optimization study on the example of a fast highly endothermal reaction aiming for an increased space-time-yield as well as a more energy efficient reactor concept was performed. The bottleneck of this reaction carried out in a multi-tubular packed bed reactor is the heat transfer into the catalyst bed. The endothermicity of the reaction results in cold spots in the center of the bed, leading to a decrease in reaction rate and thus reduced overall conversion. In tubular reactors, suitable heating profiles along the reactor axis can be realized by different options. An optimization study considering varying catalyst bed composition, alternative heating methods as well as structured catalysts was performed. Novel catalyst support structures, e.g. so-called Periodic Open Cellular Structures (POCS) as introduced by Freund, Schwieger and coworkers (Inayat et al., 2011), wash-coated with catalyst have proven to significantly increase the overall heat transfer in the reactor. Adding conventional catalyst pellets into the void space of the POCS, known as packed POCS (Ambrosetti et al., 2020), maximizes catalyst inventory while maintaining a high overall heat transport. The goal of this study is to determine optimization possibilities of the industrial reactor by intensifying the heat transport into the catalyst bed, thereby becoming more energy-efficient while achieving a higher space-time-yield.

Reference Reactor Model

A reference case of an industrial multi-tubular reactor for the exemplary reaction was simulated. The high endothermicity of the reaction leads to a large temperature difference at the reactor inlet between the reactor wall and the center of the catalyst bed. The influence of the weight hourly space velocity (WHSV) on the overall

conversion and the temperature profile along the reactor axis was investigated to determine the limitations of the current reactor setup (see Figure 1).

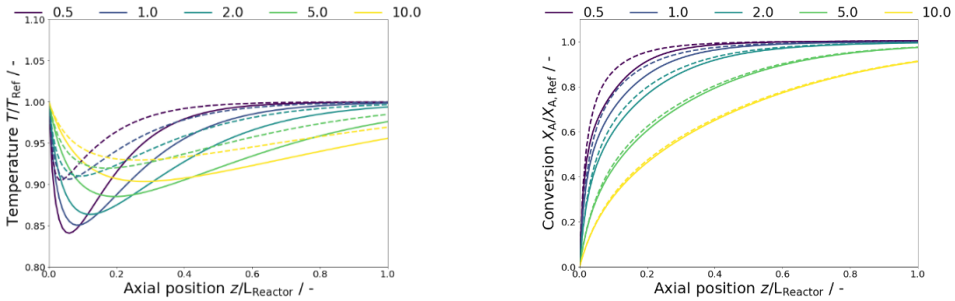

Figure 1: Temperature (left) and conversion (right) profiles of the reference reactor showing the influence of the weight hourly space velocity varied in a range of $\mathrm{WHSV}/\mathrm{WHSV}_{\mathrm{Ref}} = 0.5 - 10$. The dotted line displays the results at the reactor wall and the solid line the values at the center of the catalyst bed.

Optimization Study with Focus on Intensified Heat Transport

The reactor optimization study was performed in two approaches. The first was a two dimensional pseudohomogeneous optimization of the existing packed bed by adding inert material (i.e., different levels of bed dilution), varying the heating temperature in different zones or a combination of these two options. Here, an optimal length of the heating zones as well as composition of the catalyst bed were determined. The second approach focusses on different reactor concepts including novel structured catalyst supports such as POCS and packed POCS. These were optimized with a one dimensional reactor model. Finally, the different optimization approaches were compared and evaluated regarding the overall conversion of the reactant and the resulting maximum productivity.

Conclusions

The optimization studies highlight different possibilities to increase the heat transport into the catalyst bed. Inserting packed POCS into the tubular reactor offers the most promising results due to the high heat transfer coefficient caused by the continuous metal structure. This leads to an increasing cold spot temperature and to a higher temperature level at the reactor outlet for high WHSVs. Consequently, a higher overall conversion can be achieved, thereby increasing the productivity and the energy efficiency of the process.

References

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