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2D Optimization of tubular reactors: A novel conceptual design tool

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Highlights

- Introduction of new conceptual design tool for process intensification
- Numerical reactor design based on dynamic optimization
- Decision basis for investigation of alternate/novel reactor concepts

1. Introduction

Highly efficient chemical reactors are fundamental for the resource- and energy-efficient production of chemicals. To enable high reactor efficiencies, the reactor design aims to realize optimal reaction conditions (e.g. the reaction temperature) along the reaction route [1].

In catalytic fixed-bed reactors, the reaction conditions along the reactor axis can be manipulated by diverse options, such as the introduction of an axial profile for the catalyst bed dilution [2]. During the model-based reactor design, this concept can also be applied to the radial coordinate of the reactor to enhance reactor performance. This concept of a 2D optimization of the catalyst bed provides a decision basis regarding alternate and impulses regarding novel reactor design configurations best suited to approximate the axial and radial profiles of the chosen design variables (e.g. particle size, dilution of the catalyst bed).

In this contribution, the potential of additionally considering control variables along the radial coordinate during the reactor design is considered via a mathematical optimization study. The catalyst bed dilution is chosen as control variable. The air-based production of ethylene oxide is investigated as a case study. The conversion of ethylene X_E is set as the objective function while lower limits for the selectivity towards ethylene oxide ($S_{E,EO} \geq 81$ %) and the space-time yield ($STY \geq 0.27$ mol m^{-3} s^{-1}) serve as additional reactor performance constraints. Furthermore, it is shown that radial optimized profiles can be used as an indicator for suitable alternate reactor concepts.

2. Methods

For the formulation of the optimization problem, the steady-state reactor balance equations are discretized via orthogonal collocation on finite elements for the axial direction and via the finite volume method for the radial direction. AMPL in combination with IPOPT 3.11 is used to solve the resulting large-scale dynamic optimization problem.

To reduce the computational effort, pseudo-homogeneous reactor balance equations are used while the solutions of the catalyst pellet balance equations are approximated via analytical expressions.

A comparison between the results of a radial optimization, an axial optimization (state-of-the-art) and a 2D optimization of the catalyst bed dilution demonstrates the potential of including the radial coordinate as an additional degree of freedom in the design of the reactor.

3. Results and discussion

In Figure 1, the profiles of the volumetric catalyst bed dilution (100% = only inert particles) as well as the resulting temperature field in the reactor are shown for the three investigated cases.

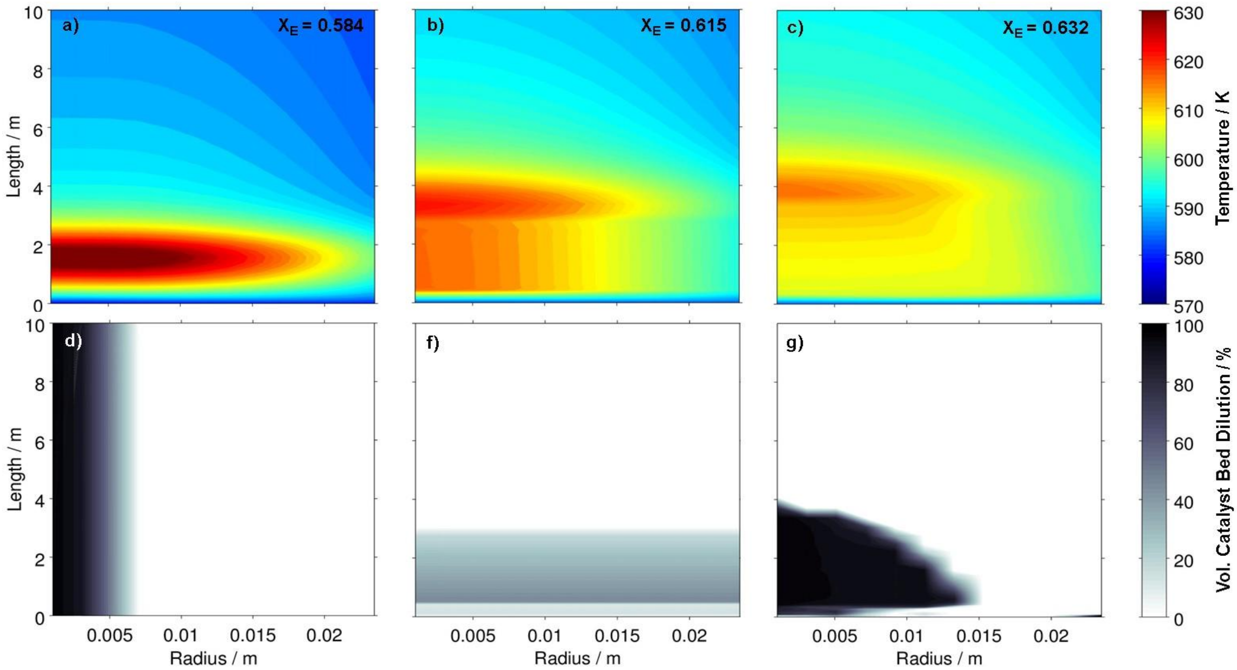

Figure 1: Top: Temperature profiles in axial and radial reactor coordinate for radial (a), axial (b) and axial&radial (c) optimized system. Bottom: Volumetric catalyst bed dilution profiles for radial (a), axial (b) and axial&radial (c) optimized system.

For the EO reaction system (kinetics according to Al-Saleh et al. [3]), there is a trade-off between high selectivity and high reaction rates, leading to an optimal reaction temperature depending on the required reactor performance constraints. This temperature can be best approximated by a combination of an axial and radial catalyst bed dilution profile, resulting in the highest conversion. As for the sole radial optimization, the lowest conversion was achieved due to the greatest inhomogeneity in the temperature profile.

However, the obtained radial dilution profile can be used as an indication in regard of other reactor concepts that approximate the resulting trends, including an estimate regarding the system performance enhancement. As for the presented case, the resulting radial dilution profile could alternatively be approximated by a tube-in-tube reactor, as it was investigated in [4]. Hence, the general concept of the radial optimization is suitable as a tool to identify or develop novel reactor types that approximate the obtained radial profiles of the chosen control variable.

4. Conclusions

The 2D optimization of catalytic fixed-bed reactors is presented and demonstrated using the ethylene oxide synthesis as case study. The obtained results visualize the optimal distribution for the investigated design variable and thereby provide guidelines and a decision basis for reactor design. In this regard, it is shown that the general concept of the radial optimization can be used as a conceptual design tool to identify or even develop innovative reactor concepts. For the considered case study, the potential of including a radial catalyst bed dilution profile was demonstrated by an increase in the conversion of ethylene by 2.8 % compared to a conventional axial dilution profile, while all other reactor performance constraints are fulfilled.

References

[1] A. Peschel, H. Freund, K. Sundmacher, Ind. Eng. Chem. Res. 49 (2010) 10535–10548.
[2] S. Hwang, R. Smith, Chem. Eng. Sc. 59 (2004) 4229-4243.
[3] M. Al-Saleh, M. Al.Ahmadi, M. Shalabi, Chem. Eng. J. 37 (1988) 35-41.
[4] A. Peschel, F. Karst, H. Freund, K. Sundmacher, Chem. Eng. Sc. 66 (2011) 6453-6469.

Keywords
Chemical reactors, Catalyst bed dilution, Reactor optimization, Process Intensification