

2D OPTIMIZATION OF INNOVATIVE REACTOR CONCEPTS VIA A NOVEL DYNAMIC OPTIMIZATION APPROACH

Alexander Pietschak¹, Andreas Brix², Hannsjörg Freund²

¹ Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Institute of Chemical Reaction Engineering, Egerlandstr. 3, 91058 Germany

² TU Dortmund University, Reaction Engineering and Catalysis, Emil-Figge-Str. 66, 44227 Dortmund, Germany
e-mail: andreas.brix@tu-dortmund.de

Keywords: Model based reactor design, 2D optimization, structured catalysts

For the resource and energy efficient production of chemicals, highly efficient reactors are of utmost importance. For this purpose, the reactor design aims to enact optimal reaction conditions along the reaction route [1].

In catalytic tubular reactors, suitable reaction conditions along the reactor axis can be promoted by diverse options such as, e.g., the introduction of an axial catalyst bed dilution profile [2]. As an extension of this concept, a profile along the radial coordinate of the reactor can simultaneously be applied to further enhance the performance. The resulting 2D optimization profiles provide a valuable decision basis as orientation for the potential of alternate and novel reactor design concepts. One such promising concept is the application of structured catalyst supports in the form of catalytic foams or tailor-made additively manufactured POCS [3].

In this contribution, the potential of additionally considering control variables along the radial coordinate during the reactor design is demonstrated via a numerical optimization study of the air-based production of ethylene oxide. The catalyst bed dilution and heat conductivity of the catalyst support are chosen as control variables. The conversion of ethylene is set as objective function while product selectivity and space-time yield serve as performance constraints.

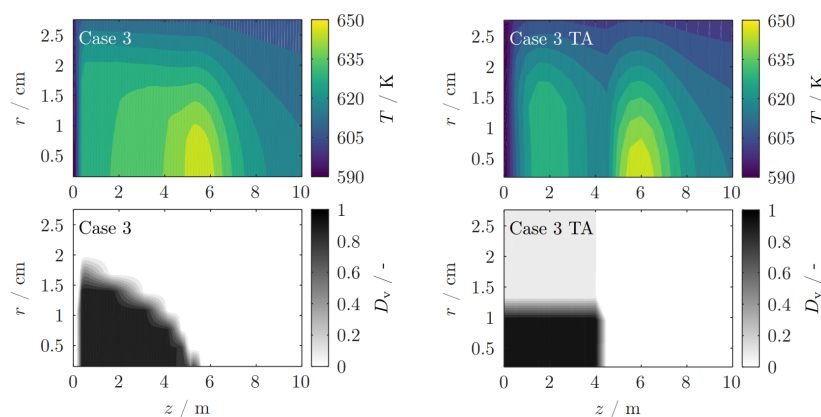


Fig. 1. Temperature profiles (Top) and catalyst bed dilution (bottom) in axial and radial direction for the optimized system (Case 3) and the technical approximation (Case 3 TA).

References

1. A. Peschel, H. Freund, K. Sundmacher, *Ind. Eng. Chem. Res.*, 2010, **49**, 10535.
2. S. Hwang, R. Smith, *Chem. Eng. Sci.*, 2004, **59**, 4229.
3. A. Inayat, J. Schwerdtfeger, H. Freund, C. Körner, R. Singer, W. Schwieger, *Chem. Eng. Sci.*, 2011, **66**, 2758.