Hierarchical modeling and analysis of heat transport properties in micro packed bed reactors

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Highlights

- Hierarchical analysis of micro packed bed reactors
- Fundamental CFD simulation of thermal behavior of packed bed reactors
- Analysis of micro packed beds under reactive conditions

1. Introduction

Fundamental multi-scale modeling of chemical reactors is considered to be one of the most promising frontiers for chemical reaction engineering and is becoming a very powerful tool for the analysis and design of novel catalytic reactors [1]. This approach is based on the multiscale simulation of the reactor behavior by means of parameters and descriptors, which are directly linked to theoretical accessible phenomena. This approach, however, is intrinsically hampered by the required computational time, which might be very demanding even for simple cases. Thus, routinely reactor analysis and design relies on simplified models based on lumped parameters, which depends on an empirical understanding of the involved phenomena. As such, their validity is often limited to the experimental conditions considered for their derivation. A promising and convenient solution to this problem is represented by the application of hierarchical approaches [2]. Detailed and computationally demanding analyses – based on Computational Fluid Dynamics (CFD) simulations – are used to study a selected number of conditions. Then, lumped parameters ready to be used in conventional reactor models are derived from CFD results. In this contribution, we use CFD for the assessment and derivation of engineering correlations by analyzing the external heat transfer coefficients in micro packed bed reactors, which have been proposed as a promising alternative to the multi-tubular fixed bed reactors for highly exothermic processes. By using the CFD-derived correlations, we analyze and compare the performances of this reactor technology applied to a selective oxidation.

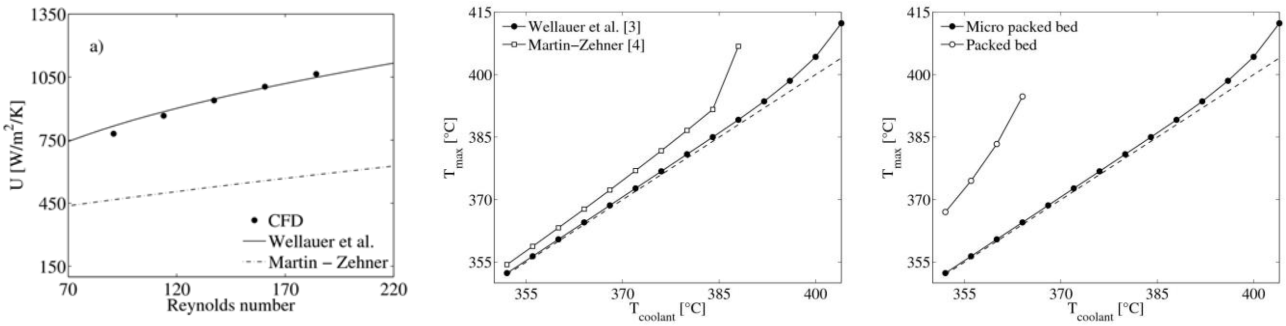
2. Methods

The analysis is based on hierarchical model to model comparison following the approach reported in [2]. The hierarchical analysis of the external heat transfer is performed by CFD simulations of heat transfer in the honeycomb matrix packed with spherical particles. By assuming identical conditions in each channel of the honeycomb, the simulation of the energy transfer in a single channel is representative of the behavior of the entire reactor. CFD simulations of the single channel are carried out by using the *chtMultiRegionSimpleFoam* solver of in the OpenFOAM framework, which describes the transport of heat and momentum in the fluid and the heat transport in the solid. Then, the CFD results are analyzed with a 1D pseudo-homogeneous model to estimate the overall heat transfer coefficients which are compared with literature correlations [3,4]. Finally, the hierarchically derived correlation is exploited in a 2D pseudo-homogenous model to analyze the selective oxidation of o-xylene to phthalic anhydride.

3. Results and discussion

We start with the analysis of predictions of the literature correlations for the overall heat transfer coefficients applied to micro packed bed reactors. The CFD analysis shows that the overall heat transfer coefficient estimated with the correlations proposed by Wellauer et al. [4] accurately describes the reactor behavior, as shown in Figure 1(a). This is line with the fact that it is derived for low Reynolds number (~70), which is the

typical flow regime for micro packed bed reactors. Then, we analyzed the conversion of o-xylene to phthalic anhydride as a case study of industrial relevance. Our analysis points out that the choice of the correlation strongly influences the prediction of the reactor behavior. By comparing the results obtained with the two correlations, temperature differences are observed within the reactor due to the different estimation of the heat transfer coefficients, as shown in Figure 1(b). The correlation proposed by Martin and Zehner [4] overestimates the temperature in the reactor and predicts the reactor runaway at lower temperature. Thus, the CFD-driven identification of the adequate correlation enables the assessment of the reliability of such reactor configuration by means of low hierarchy models which fully retain the characteristic features observable with the fundamental approach. This allows for a comprehensive analysis of the effect of the operating conditions on the performances of micro packed beds. The simulation of the phthalic anhydride micro packed bed reactor shows higher heat transfer properties than a multi-tubular packed bed reactor. The micro packed bed is almost isothermal even if the same yield as the packed bed is achieved. Moreover, the 2D model, with the hierarchically derived correlation, shows the capability of an increase of the coolant temperature in the micro packed bed reactor up to 404 °C, as shown in Figure 1(c), by keeping the maximum temperature in the reactor below the catalyst deactivation limit and increasing the overall yield of the process. This result seems to overcome the performances of industrial packed bed reactors that expects runaway with coolant temperature around 360 °C.



(a) (b) (c)

Figure 1. Comparison between external heat transfer coefficients evaluated with CFD and literature correlations [3,4] (a); maximum temperature in micro packed bed predicted with different correlations [3,4] (b); maximum temperature in the reactor for micro packed bed and industrial reactor (c)

4. Conclusions

By using CFD, we proved that the correlations proposed by Wellauer et al. [4] appropriately describe the behavior of micro packed bed reactors. We assessed the effect of the selected correlation on the performances of the reactor, showing that the proper description can be effectively achieved with hierarchically-derived information. Finally, we showed the capabilities of micro packed bed reactor to overcome the limitation of industrial packed reactor enabling the operation at higher yields.

Acknowledgments

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Keywords
micro packed bed reactor; hierarchical approach; process intensification; heat transfer