HIERARCHICAL ANALYSIS OF THE GAS-TO-PARTICLE HEAT AND MASS TRANSFER IN MICRO PACKED BED REACTORS

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Abstract

A hierarchical approach for an efficient exploitation of fundamental multi-scale modeling for the analysis and design of the kinetic-transport interactions in chemical reactors is proposed. In essence, detailed results, obtain with Computational Fluid Dynamics simulations (CFD) of the reactor, are interpreted by means of 1D heterogeneous models. This approach allows for the derivation of lumped parameters, which are related to a detailed and sound description of the governing phenomena. The very good agreement between the predictions of CFD and 1D heterogeneous models at different operating conditions shows that the CFD-based correlations for transport properties fully retains all the main features of detailed CFD simulations. Therefore, on a more general basis, this work clearly demonstrates the potentiality of the hierarchical application of CFD simulation for the derivation of transport parameters in reactor engineering, which can be used for the efficient and fundamental analysis and design of novel reactor technologies.

Keywords

Micro packed beds; Hierarchical modeling

Introduction

Fundamental multi-scale modeling of chemical reactors is considered as one of the most promising frontiers for chemical reaction engineering (Dudukovic, 2009), but it is intrinsically limited by the required computational time. In fact, it cannot be applied in routinely reactor analysis and design, which have still to resort to simplified and lumped models, which are based on an empirical understanding (Froment et al., 1990). For this reason, their validity is often limited to the experimental conditions considered for the derivation.

A promising and convenient solution to this problem is represented by the application of hierarchical approaches, where detailed methods – based on Computational Fluid Dynamics simulations (CFD) – are first used to study a selected and limited number of conditions. Then, CFD analyses are interpreted for the derivation of lumped parameters to be adopted in classical reactor modeling (Logtenberg and Dixon, 1998).

This approach can be particularly useful in the analysis and design of novel micro-reactor configurations, such as micro packed bed reactors, which have been proposed as a promising alternative to the multi-tubular fixed bed reactors for highly exothermic reactions (Holladay et al., 2004). These micro packed beds consist of catalytic spheres with diameter of the order of 500 μm, which determines operating conditions very different from the ones of conventional industrial packed bed reactors (Vervloet et al., 2013). Therefore, there is no guarantee that the state-of-the art correlations developed for packed

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beds can be extended to this context and a detailed and fundamental assessment is required.

At this scope, here we propose and apply a hierarchical approach to analyze the gas-to-particle heat and mass transfer in micro packed bed reactors and to assess the validity of existing transport correlations for the analysis and design of micro packed beds.

Methods

Different models and methods are employed for the application of the hierarchical methodology to the analysis of the transport properties in micro packed beds. At the highest hierarchy level the random packing is generated by means of Discrete Element Method (DEM) and the detailed analysis of the transport properties is performed with CFD simulations. Then, the CFD results are interpreted by means of 1D heterogeneous, steady state models, where lumped parameters are implemented (lowest level of hierarchy).

Results

Three different micro packed beds with different tube-to-particle diameter ratio are generated and their transport properties in terms of mass and heat transfer coefficients are analyzed.

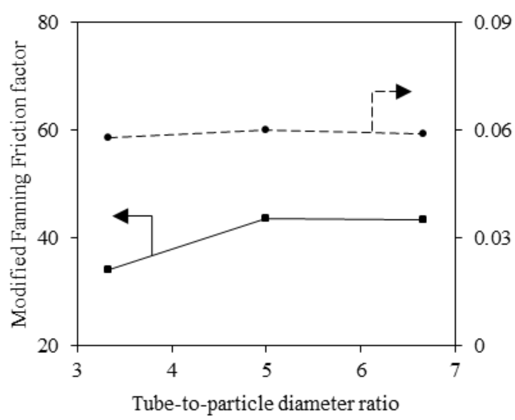

Figure 1. Comparisons of the dependence on tube-to-particle diameter ratio of the Modified Fanning friction factor and the j-factor

The analysis shows that there is no substantial difference between the j-factors for heat and mass transfer in agreement with the Chilton-Colburn analogy. Moreover, as show in Figure 1 wall effects have no impact on the estimation of the j-factor, contrary to pressure drops.

Finally, based on the CFD simulations, we derive a suitable correlation, whose results are similar to those estimated by literature correlations in the same flow conditions, as reported in Figure 2.

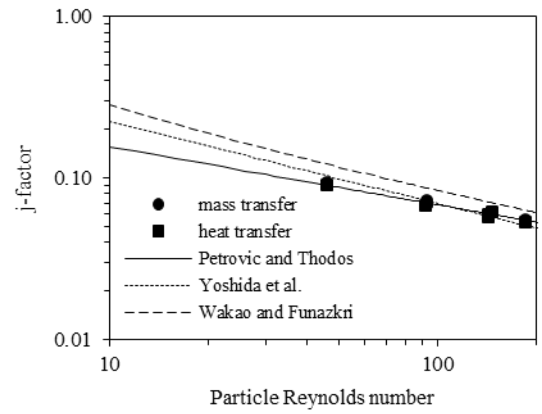

Figure 2. Heat and mass transfer properties: comparison between the computer-generated packed beds and the correlations from literature

This comparison supports the reliability of the hierarchical approach and shows that it can be conveniently used for the derivation or validation of correlations in different conditions. In particular it can be very helpful in the analysis of micro-reactor technologies.

Conclusions

The potentialities of the hierarchical approach for modeling transport phenomena in catalytic reactors have been proven by the investigation of the gas-to-particle mass and heat transfer in micro packed bed reactors.

CFD simulations are used to hierarchically derive a transport correlation for micro packed beds. This correlation resulted to be very similar to literature ones, which are experimentally derived on beds of typical industrial scale in the same flow conditions. This work clearly demonstrates the potentiality of the hierarchical derivation of transport parameters in reactor engineering, which can be employed for the efficient and fundamental analysis and design of novel reactor technologies

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