Chemical Engineering Journal 289 (2016) 471–478

Contents lists available at ScienceDirect

Chemical Engineering Journal

journal homepage: www.elsevier.com/locate/cej

Hierarchical analysis of the gas-to-particle heat and mass transfer in micro packed bed reactors

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HIGHLIGHTS

- A CFD-based hierarchical approach for lumped parameter derivation is proposed.
- This approach allows to efficiently exploit CFD simulations in reactor modeling.
- Gas-to-particle transport phenomena in micro packed bed reactors are analyzed.
- Literature correlations for gas-to-particle transport in packed beds are assessed.

ARTICLE INFO

Article history:
Received 24 October 2015
Received in revised form 20 December 2015
Accepted 21 December 2015
Available online 2 January 2016

Keywords:
Micro packed beds
Mass transfer
Heat transfer
Gas–solid catalytic reactor
Hierarchical modeling
CFD

ABSTRACT

In this paper we propose and apply 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. In essence, detailed and computationally demanding analyses – based on computational fluid dynamics simulations (CFD) of the reactor – are first used to study in detail a selected and limited number of conditions. Then, the CFD results are interpreted by means of 1D heterogeneous models for the derivation of lumped parameters to be used in classical reactor models. On one side, this approach limits the use of computationally demanding simulations. On the other side, it allows for the rational derivation of 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 correlation for transport properties fully retains all the main features of the detailed CFD simulation. Moreover, we found that the hierarchical derived correlations to be very similar to the ones experimentally obtained for typical industrial scale packed bed reactors, thus confirming that the conventional correlations may be reliably used in micro-packed bed reactors.

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.

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1. Introduction

Fundamental multi-scale modeling of chemical reactors is considered as 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 [1,2]. 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. Such a detailed and fundamental description is crucial to help the interpretation of experiments and to allow for a rational engineering of the chemical transformation for advanced process intensification [3,4]. This approach, however, is intrinsically limited by the required computational time, which can be very demanding even for simple cases. As a consequence, it cannot be applied in routinely reactor analysis and design, which have still to resort to simplified and lumped models [5]. There, the parameters are often based on phenomenological descriptions based on an empirical understanding of the involved phenomena. As such, 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 for modeling the kinetic–transport interactions in chemical reactors.

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http://dx.doi.org/10.1016/j.cej.2015.12.089
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Notation

Latin letters

A	cross section area [m^2]
c_P	specific heat at constant pressure $\left[\frac{J}{kg\ K}\right]$
D_P	particle diameter [m]
D_T	tube diameter [m]
h	heat transfer coefficient $\left[\frac{W}{m^2\ K}\right]$
j_F	generic j-factor [–]
k	gas mixture conductivity $\left[\frac{W}{m\ K}\right]$
k_{MAT}	mass transfer coefficient of limiting reactant $\left[\frac{m}{s}\right]$
k_C	first order kinetic constant $\left[\frac{m}{s}\right]$
L	packed reactor length [m]
N	tube-to-particle diameter ratio [–]
N_P	number of sphere particles [–]
p	pressure [Pa]
S_V	area-per-unit volume $\left[\frac{1}{m}\right]$
T^B	temperature of the gas phase [K]
T^W	wall temperature [K]
u	superficial velocity $\left[\frac{m}{s}\right]$
z	reactor axial direction [m]

Subscripts

IN	inlet of the packing ($z = 0$)
OUT	outlet of the packing ($z = L$)

Greek letters

ε	void fraction [–]
ω^B	mass fraction of the limiting reactant in the gas phase [–]
ω^W	mass fraction of the limiting reactant on the catalytic wall [–]
ρ	gas phase density $\left[\frac{kg}{m^3}\right]$
Γ	diffusivity of limiting reactant in the gas mixture $\left[\frac{m^2}{s}\right]$
μ	gas mixture viscosity $\left[\frac{kg}{m\ s}\right]$

Dimensionless numbers

$Da = \frac{k_C D_P}{\Gamma}$	Damkholer's number
$Re = \frac{\rho u D_P}{\mu}$	Reynolds' number
$Sc = \frac{\mu}{\rho\Gamma}$	Schmidt's number
$Pr = \frac{\mu c_P}{k}$	Prandtl's number
$Sh = \frac{k_{MAT} D_P}{\Gamma}$	Sherwood's number
$Nu = \frac{h D_P}{k}$	Nusselt's number
$Pe = Re\ Sc$	Péclet's number for mass transfer
$Pe = Re\ Pr$	Péclet's number for heat transfer
$j_M = \frac{Sh}{Re Sc^{1/3}}$	j-factor for mass transfer
$j_H = \frac{Nu}{Re\ Pr^{1/3}}$	j-factor for heat transfer
$f_m = \frac{\Delta p}{L}\frac{D_P}{\rho u^2}$	modified Fanning friction factor

A schematic of the methodology is reported in Fig. 1. In essence, accurate methods – based on computational fluid dynamics simulations (CFD) of the detailed reactor geometry – are first used to study in detail a selected and limited number of conditions. Then, CFD analyses are used and interpreted for the derivation of lumped parameters to be adopted in classical reactor modeling [6–9]. On one side, this approach limits the need of computationally demanding simulations. On the other side, it allows for the rational derivation of parameters, which are related to a detailed and sound description of the governing phenomena by means of novel or refined correlations for the estimation of the transport coefficient. This approach can be particularly useful in the analysis and design of novel micro-reactor configurations, where the classical correlations for the evaluation of transport coefficients are not yet established and validated. In this respect, the hierarchical analysis by means of CFD simulations can allow for a sound analysis and assessment of the parameters, which have been derived at different operating conditions and reactor configurations. For instance, this is the case of micro packed bed reactors, which have been proposed as a promising alternative to the multi-tubular fixed bed reactor for highly exothermic reactions [10,11]. On one side, correlations and parameters for modeling packed bed reactors are considered as widely validated in typical industrial conditions [5]. On the other side, these micro packed beds consist of catalytic spheres with diameters of the order of 500 μm, as shown in Fig. 2. This leads to operating conditions and geometries of the bed very different from the ones of conventional industrial packed bed reactors [10,12,13]. Therefore, there is no guarantee that the state-of-the art correlations developed for packed beds can be extended to this context and a detailed and fundamental assessment is required.

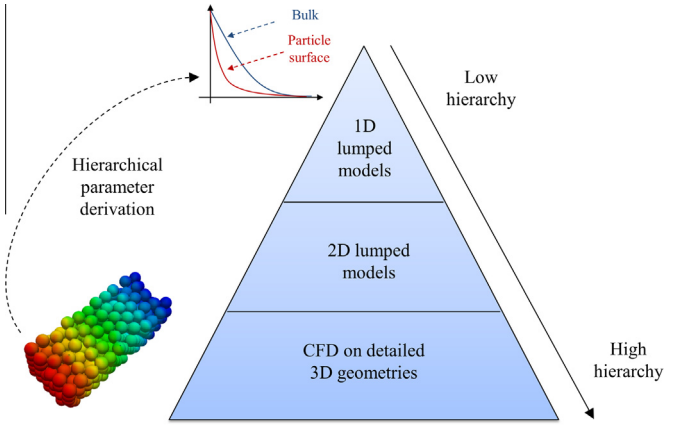

Fig. 1. Schematic description of the hierarchical approach. Results from fundamental multiscale models are analyzed with lower hierarchy models and lumped parameters are derived.

At this scope, here we propose and apply a hierarchical approach (i) to analyze the gas-to-particle heat and mass transfer in micro packed bed reactors and (ii) to assess the validity of existing transport correlations for the analysis and design of micro packed beds. First, we perform a detailed CFD analysis of heat and mass transport on different geometries of micro-packed beds at different tube-to-particle diameter ratio, thus accounting also for the effect of channeling, which can be a major issue in this reactor configuration [10]. Such an analysis is then interpreted by means of 1D heterogeneous models of the reactor in order to develop suitable correlations for the gas-to-particle heat and mass transfer properties in micro packed bed reactors. We show that there is no substantial difference between the heat and mass transfer, as expected by the Chilton–Colburn analogy [14]. Our results reveal that the dimension of the particle is not determining and

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