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Numerical up-scaling approach for the simulation of heat-transfer in randomly packed beds

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ABSTRACT

The objectives of this paper is to report the development and validation of a computational fluid dynamics (CFD) modeling approach to predict heat transfers in arbitrary randomly packed tubular reactors. The capacity of the packed beds to supply or remove heat from the core to the tube walls is indeed critical for the performance of reactors involved in various chemical applications of catalytic reactions. The understanding of the physical mechanisms and the modeling of turbulent heat and mass transfer is thus essential for the design, optimization and scale-up of fixed-bed reactors.

For this objective, the heterogeneous catalyst bed can be represented by a macroscopic or homogeneous one where turbulence does exist at the small scales. In this study, an up-scaling approach is considered where the volume averaging procedure is used to derive the macroscopic equations. The flow and turbulent variables are decomposed according to the double decomposition concept within the framework of the volume averaging method. In particular, the dispersive kinetic energy is considered for the modeling of the thermal dispersion term appearing in the macroscopic temperature equation with a k–ε approach. The model is extended for the prediction of the channeling effects near the tube walls. The closure approximations are validated with microscopic simulations performed at the scale of representative elementary volume and comparisons with macroscopic simulations. Several packed bed configurations are considered, and the model predictions for the core heat transfer and the wall heat transfer are also compared to usual correlations when available.

The microscopic simulations performed for various particle shapes are also confirming the predominant contribution of the mechanical dispersion to the convective heat transfer.

This study is demonstrating the feasibility to predict the global heat transfer inside arbitrary tubular reactors with simple macroscopic simulations as an alternative to complex and computationally expensive microscopic simulations, out of the range of usual engineering tasks.

1. Introduction

Fixed bed reactors are widely used processes in various chemical applications involving catalyst reactions. The usual fixed-bed reactor or tubular reactor is based on a cylindrical tube which is randomly filled with catalyst particles. For practical applications, the typical particulate Reynolds number of the flow inside the tubular reactor based on average superficial velocity and average particle diameter can range typically between 1000 and 10,000 and the flow can then be considered as a fully turbulent flow. Reactions can be endothermic or exothermic, and the performance of tubular reactors regarding heat transfers can be critical to supply or remove heat from the reactor bed. The understanding of the physical mechanisms of heat and mass transfer is thus essential for the design, optimization and scale-up of fixed-bed reactors.

Recent advances in the application of the computational fluid dynamics (CFD) to the modeling of heat and mass transfer in fixed beds [1] have demonstrated the benefit of such simulations for a better understanding of the physical mechanisms. These simulations performed at the microscopic scale remain however expensive in particular due to the complexity of the geometry and of the coupled physics and cannot be easily considered to represent the flow inside a complete tubular reactor.

On the contrary with the recent developments regarding up-scaling approaches combining the averaging procedure [23,24] and the double decomposition technique [4], it is possible to envisage macroscopic simulations at the scale of the complete reactor with a more realistic representation of the physics than the usual plug flow approximation based on ad-hoc correlations, in particular for innovative geometries for which such correlations are not available.

The objective of this paper is to report the work in progress regarding the development of an up-scaling approach to model

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Notations

α_w	wall heat transfer coefficient (W/m^2/K)
α_w^0	wall heat transfer coefficient – stagnant contribution (W/m^2/K)
C_p^f	specific heat of fluid at constant pressure (J/Kg/K)
c_{mu}, c_k, c_ε, σ_t	turbulence model coefficients
dp	diameter of the catalyst particle (or pellet) (m)
d_{tin}	tube inner diameter (m)
d_{tou}	tube outer diameter (m)
ε	macro-scale turbulence dissipation rate (m^2/s^3)
γ	packed bed porosity
k	macro-scale turbulent kinetic energy (m^2/s^2)
k_M	large scale turbulence kinetic energy (m^2/s^2)
k_m	small scale turbulence kinetic energy (m^2/s^2)
k_{dis}	dispersive kinetic energy (m^2/s^2)
κ	heat transfer rate in the core flow
λ_{eff}	radial effective conductivity (W/m/K)
λ_{eff}^0	stagnant radial effective conductivity (W/m/K)
λ_{eff}^{0s}	solid contribution to the stagnant radial effective conductivity (W/m/K)
λ_{eff}^{0f}	fluid contribution to the stagnant radial effective conductivity (W/m/K)
λ_{eff}^{conv}	convective contribution to the radial effective conductivity (W/m/K)
λ_{eff}^*	normalized radial effective conductivity with the fluid conductivity
λ_f	fluid conductivity (W/m/K)
λ_s	solid conductivity (W/m/K)
λ_t	tube conductivity (W/m/K)
Nu	Nusselt number
ν_f	molecular fluid kinematic viscosity (m^2/s)
ν_t	turbulent fluid kinematic viscosity viscosity (m^2/s)
Re	particulate Reynolds number (Re = $\rho V_s d_p/\mu_f$)
Pe	Peclet number (Pe = Re · Pr)
p	solid emissivity
Pr	fluid Prandtl number
Q	wall heat flux (W/m^2)
ρ	fluid density (kg/m^3)
S^*	tube specific surface (1/m)
σ_T	macroscopic turbulent Prandtl number
T	temperature (K) in the porous media
T_W	temperature (K) at the inner tube wall
$\bar{\vartheta}$	time averaged quantities
ϑ'	time fluctuation
$\langle\vartheta\rangle^i$	spatial average
${}^i\langle\vartheta\rangle$	spatial deviation
$\boldsymbol{u}$	fluid velocity vector (m/s)
u, v	fluid velocity component (m/s)
U_1	global heat transfer coefficient without tube wall resistance (W/m^2/K)
U_2	global heat transfer coefficient including tube wall resistance (W/m^2/K)
V_s	superficial (or Darcy) velocity (m/s)
x, r	axial and radial direction

the turbulent heat and mass transport in arbitrary reactor configurations with CFD. At the macroscopic scale, effective thermal properties both under stagnant conditions and with the turbulent convection are modeled separately. The simplified model of Kunii and Smith [12] is considered to represent the effective conduction and radiation in porous media under stagnant conditions since it is not the main contribution to heat transfer at high Reynolds numbers. A novel approach is considered to model the turbulent convective heat and mass transport based in particular on a new definition of the macroscopic turbulent kinetic energy [27]. Indeed, dispersion terms appearing in the energy equation are presumably not negligible due to the relatively low porosity of the media. In this study the thermal dispersion is modeled through a gradient diffusion hypothesis and the consideration of a constant macroscopic turbulent Prandtl number [5]. The scope of the study is also to address the modeling of the channeling effects near the walls with the consideration of a two layer k–ε modeling approach.

Micro-scale numerical simulations of the hydrodynamic flow are considered to compute the model coefficients on a representative elementary volume of the packed bed. Similar to the turbulent modeling approaches based on filtering operations, the models are validated thanks to "a priori" and "a posteriori" tests [7] of prototype porous media flow configurations. Usual experimental correlations are also considered to validate the prediction of the radial heat transfer in the core of the packed bed reactor and the prediction of the wall heat transfer, at low and high temperature ranges.

The concept of the up-scaling approach is briefly introduced in the first part of the paper. The macroscopic equations and the macroscopic models considered to represent momentum and heat transfers are then detailed in the two next sections. The determination of the model coefficients and the validation performed regarding the prediction of the effective conductivity and the wall heat transfer are then reported in the last parts of the paper.

During this study, the commercial software Fluent was used to perform both the microscopic and the macroscopic simulations. A full description of the numerical schemes and models is given in [31].

2. Up-scaling approach for heat transfer modeling

Despite the fact that it might be possible to describe some packed beds in an almost exact representation at the microscopic scale with computational fluid dynamics (CFD) or with a meaningful approximation of the geometry [21], the computational effort required to solve the complete flow and temperature field in for instance a complete tubular reactor is still out of reach for practical engineering simulations. Moreover the primary interest for industrial purposes is not the details of the flow but the knowledge at a larger scale of mean flow quantities and heat transfer properties. This motivates the development of porous media approximations such as originally developed for micro-porous flows [25]. In the present case the heterogeneous catalyst bed is represented by a macroscopic or homogeneous one where turbulence does exist at the small scales.

In this case suitable approaches to model turbulence and heat transfer at the macroscopic scale need to be developed. For instance, an up-scaling approach [23] can be considered where the volume averaging procedure is used to derive the macroscopic equations. This averaging procedure leads to a set of modified equations for the mean flow quantities with additional contributions which account for the small scales effects on the macroscopic velocity and temperature field.

The closure approximations for these additional terms can be derived by considering a representative elementary volume (REV) of the packed bed. For complex geometries and turbulent flows for which analytical solutions are not available, heat and