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Simulation of heat transfer and hydrodynamics for metal structured packed bed

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Abstract

Modeling and simulation based on computational hydrodynamics and heat transfer for metal structured packed bed are carried out to predict the flow field and temperature field, and to evaluate its performance in transport aspect. The comparison between the simulation results for the metal structured packed bed and the experimental heat transfer performance as well as pressure drop of the conventional pellet packed bed is made, which quantitatively validates that transport performance of the metal structured packed bed is much better. Furthermore, the effects of geometric parameters and the property of solid phase on heat transfer of the metal structured packed bed are discussed. It is found that at low *Re*, the specific surface area is a key factor to determine the heat transfer capability of the structured bed. However, when *Re* turns to be high, the property of solid phase and voidage of the structured packed bed will play an important role in the evaluation of its heat transfer. In light of above results, some feasible methods are available to enhance the heat transfer performance.

Keywords: Computational hydrodynamics; Metal structured packed bed; Heat transfer performance; Pressure drop

1. Introduction

Process intensification refers to the development of novel apparatuses and techniques that are expected to bring dramatic improvements in manufacturing and processing compared to those commonly used today [1]. As one of the process intensification techniques, monolith catalyst (structured catalyst) has a lot of advantages over conventional pellet catalyst in macro-kinetics of heterogeneous catalytic reactions and transport characteristics. Conventional fixed-bed reactor randomly packed with the pellets of catalyst has a poor heat transfer that can induce hot spots in exothermic reactions. The packed-bed catalytic reactor whose catalyst support is monolith, especially metal monolith, has much higher surface area per unit volume of the bed, which guarantees a good heat transfer throughout the reactor. Besides, it also offers a much lower pressure drop in comparison with the pellet packed-bed reactor. So, monolith catalyst has received much attention from academia since it came up in the 1990s late period [2]. Recently, it was gradually applied in petroleum and chemical engineering process.

The developments in the field of monolith catalyst can be found in many review articles. Valentini et al. [3] presented a fundamental experimental study on a method for preparing monolith catalyst, and the heat and mass transfer performance of monolith catalyst has been investigated to design more efficient system by experiments [4–6]. Other than experimental research, mathematical modeling and simulation have become powerful tools to predict transport and reaction performances in chemical engineering processes [7], so more and more papers about the simulation of monolith catalyst, especially about the simulation for reaction characteristics of catalytic combustion, are coming up. For example, geometry effects on ignition in a catalytic

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Nomenclature

c_g	heat capacity of the gas (J kg^{-1} K^{-1})
c_s	heat capacity if the solid (J kg^{-1} K^{-1})
d	channel diameter of the metal structured packed bed (m)
d_p	pellet diameter of the pellet packed bed (m)
e	height of the rough layer (m)
G	gas mass flux (kg m^{-2} s^{-1})
h	thermodynamic enthalpy (J kg^{-1})
h_{tot}	total enthalpy (J kg^{-1})
k	turbulence kinetic energy (m^2 K^{-2})
L	length of bed (m)
n	number of the gas (mol)
P	pressure of the gas (Pa)
Pr	Prandtl number ($C_p\mu/\lambda_g$)
r	radial bed position (m)
R	diameter of the metal structured packed bed (m)
Re	Reynolds number based on pellet packed bed ($du\rho/\mu$)
Re_p	Reynolds number based on pellet packed bed ($d_p u\rho/\mu$)
R_g	gas constant (J mol^{-1} K^{-1})
T	temperature of the gas (K)
T_w	wall temperature of bed (K)
T_0	gas temperature at inlet (K)
u	gas velocity (m s^{-1})
V	gas volume (m^3)
x	axial bed position (m)

Greek letters

Γ_{eff}	effective coefficient for energy balance equation (kg m^{-1} s^{-1})
δ	identity matrix
ε	turbulence eddy dissipation (m^2 K^{-3})
λ_{er}	radial effective conductivity of the bed (W m^{-1} K^{-1})
λ_g	thermal conductivity of the gas (W m^{-1} K^{-1})
λ_s	thermal conductivity of the solid (W m^{-1} K^{-1})
μ_{eff}	effective viscosity (kg m^{-1} s^{-1})
$\mu_{laminar}$	molecular viscosity under laminar flow (kg m^{-1} s^{-1})
$\mu_{turbulent}$	molecular viscosity under turbulent flow (kg m^{-1} s^{-1})
ρ	gas density (kg m^{-3})
σ_T	experimental constant

monolith were discussed by solving the convection–diffusion differential equations with wall reaction in the monolith having smooth geometry or sharp corners [8]. Groppi and Tronconi [9] considered the effect of catalyst design parameters by a pseudo-continuous, heterogeneous 2D monolith reactor model for highly exothermic reactions. Because catalytic combustion of methane in structured reactors is an effective and clean technology for industrial and domestic applications, a considerable amount of simulation research has been devoted to such progresses. Dupont et al. [10] have shown that catalytic combustion of methane can achieve ultra-low emissions of NO_x, CO and unburned hydrocarbons by using monolith catalyst. Veser and Frauhammer [11], Cimino et al. [12] and Chou et al. [13] developed a two-phase model to explain various steady-state and transient behaviors of structured reactors during catalytic combustion of methane. The study for hydrogen-assisted catalytic combustion of methane [14], the identification of suitable kinetic constants [15] and the discussion for the effects of operation conditions [16] and axially non-uniform catalyst distributions [17] were all carried out. The simulations of other reactions, such as catalytic combustion of carbon monoxide [18] or ammonia [19], were also reported. In the last years, a new reactor concept [20] for the coupling of exothermic and endothermic reactions was suggested. Zanfir and Gavriilidis [21] demonstrated that the ratio of catalyst loading for the two reactions is a key variable, which must be carefully adjusted to avoid hot spots or insufficient reactant conversion. The effect of operation conditions in this kind of configuration was also analyzed carefully [22]. Recently, to achieve enhanced catalytic combustion, a wire-mesh honeycomb catalyst support was constructed to substitute for the corrugated sheets packed within a frame [23]. Another support structure [24] was a three-dimensional lattice of rods created by a direct fabrication technique, and this structure generated highly turbulent flow and promoted increased mass transfer when compared to the extruded-honeycomb structure. In addition to the simulations for reaction, transport characteristics of the support of the structured catalyst were also investigated in some papers [25–27].

As we see from the above studies, most of them put emphasis on the investigation of reaction characteristics of monolith catalyst whose supports are often ceramic. Actually, the reaction performances of monolith catalyst considerably depend on transport characteristics of its support, which are reported in only a few literatures. In this work, the object is to study hydrodynamic and heat transfer performances of metal structured packed bed only filled with metal monolith supports without catalyst by using mathematical models. As well known, the heat transfer performance of the catalytic reactor using structured metal as support strongly depends on that of the structured support because the washcoat layer where active species are loaded is very thin compared with the thickness of the support wall. So, it seems to be helpful to discuss the heat transfer characteristics of metal structured packed bed filled with metal monolith support without chemical reaction and effects of geometric and operating parameters on it. In fact, based on such a work, it is easy to simulate a catalytic reactor using structured metal as support by means of adding the reaction kinetic contribution acting as source or sink into the model.