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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.

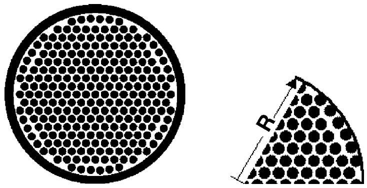

Fig. 1. The cross-section of the metal structured metal packed bed.

2. Model description

To simulate conveniently, it is assumed that the metal structured packed bed is a cylinder. As shown in Fig. 1, there are many axially parallel channels whose arrangement is correctitude triangle in the cross-section of the bed. The simulated region was chosen as one-sixth of the bed.

The flow medium is air as an ideal gas and the temperature on the external wall of the monolith is to be constant. Computational fluid dynamics (CFD) will be applied to calculate the temperature, velocity and pressure profiles and predict the steady-state performance of the bed. The model considers the flow, convective heat transfer of the gas and the conduction of the solid. A set of governing equations can be obtained, including mass, momentum and energy balances for gas phase, energy balance for solid phase, state equation for ideal gas and a correlation of viscosity with temperature for gas phase.

- Gas phase:
  Continuity equation:

$$\nabla \cdot (\rho \vec{u}) = 0 \tag{1}$$

  Momentum balance equation:

$$\nabla \cdot (\rho \vec{u} \otimes \vec{u}) = \nabla \cdot (-P\delta + \mu_{\text{eff}}(\nabla \vec{u} + (\nabla \vec{u})^{\text{T}})), \quad \mu_{\text{eff}} = \mu_{\text{laminar}} + \mu_{\text{turbulent}} \tag{2}$$

  Energy balance for gas phase:

$$\nabla \cdot (\rho \vec{u}\, h_{\text{tot}}) = \nabla \cdot (\Gamma_{\text{eff}} \nabla T), \quad \Gamma_{\text{eff}} = \lambda_{\text{g}} + \frac{\mu_{\text{turbulent}}}{\sigma_{\text{T}}} \tag{3}$$

  The value of $\mu_{\text{turbulent}}$ is taken to zero under the laminar flow, while $\mu_{\text{turbulent}}$ is calculated by solving the K–ε two-equation model that is widely used under the turbulent flow. h_{tot} is the total enthalpy, obtained by addition of the kinetic energy of the fluid to the thermodynamic contribution, h:

$$h_{\text{tot}} = h + \tfrac{1}{2}u^2 \tag{4}$$

- Solid phase:
  Energy balance for solid phase:

$$\nabla \cdot \left(\frac{\lambda_{\text{s}}}{c_{\text{s}}} \nabla T \right) = 0 \tag{5}$$

- Equation of state for ideal gas:

$$PV = nR_{\text{g}}T \tag{6}$$

- Correlation of viscosity with temperature for gas phase [28]:

$$\mu = (8.9376 \times 10^{-6}) + (0.035672 \times 10^{-6})\, T \tag{7}$$

In the balance equations above, density is allowed to vary with T and P according to the state equation of ideal gas. Buoyancy and heat flux by radiation are neglected. To solve the governing equations, appropriate boundary conditions must be specified at all external boundaries. The following assumptions are adopted for determining boundary conditions:

(1) uniform gas velocity and temperature at the entrance;
(2) fully developed gas velocity and temperature at the outlet;
(3) invariable and uniform temperature at the external wall of the bed, no slip conditions at the wall of the channel;
(4) axial adiabatic solid boundary at the entrance and the outlet.

The commercial code used in this study is CFX of AEA Technology. The technique of finite volume is used to discrete the governing equations. The equations for gas phase are solved combined with solid phase equations. The resulting structural mesh for the bed has approximate 10^5 tetrahedron cells. Solving the above equations can get temperature and velocity profiles in the bed.

3. Results and discussions

3.1. The comparison with pellet packed bed

3.1.1. The comparison by using effective heat transfer parameter

In order to show the advantages of metal structured packed bed in heat transfer, we will make a comparison in the performance of heat transfer between the simulated results for metal structured packed beds and the experimental results for a pellet packed bed which has been obtained in our research group before, in terms of radial effective heat conductivity.

The packings in the experimental pellet packed bed were ringed catalyst supports with inner diameter 1.3 mm, outer diameter 5.5 mm and height 5.5 mm, whose volume-equivalent diameter is 5.6 mm. To compare with this pellet packed bed, a metal structured packed bed, marked as 1–1, with the same voidage as the pellet packed bed is simulated. Moreover, the simulation conditions are also the same as the experimental conditions of this pellet packed bed. The specific structure parameters and operation conditions are shown in Table 1. At the same time, those of another metal structured packed bed, marked as 2–1, are also listed in this table to compare heat transfer performance between different metal structured packed beds.

Table 1
The experimental and simulation conditions, and structured parameters for the pellet packed bed and the structured metal packed beds, respectively

Object	Experimental pellet packed bed	Structured metal packed bed 1–1	Structured metal packed bed 2–1
Name of the packing	Ringed	Structured	Structured
Material of packing	γ-Al_2O_3	Aluminum	Aluminum
Fluid medium	Air	Air	Air
Equivalent diameter of pellet (m)	0.0056	/	/
Aperture diameter (m)	/	0.0024	0.002
Diameter of bed (m)	0.035	0.035	0.035
Height of bed (m)	0.742	0.450	0.500
Voidage of bed	0.395	0.399	0.278
Specific surface area (m^{-1})	642.48	66612	55510
Range of fluid flux (kg m^{-2} s^{-1})	3.78–8.18	2.02–9.61	2.11–7.90
Gas temperature at inlet (°C)	200.0	200.0	200.0
Wall temperature of bed (°C)	370.0	370.0	370.0

So far, a widely adopted method to describe radial heat transfer of conventional pellet packed bed is to use a stationary pseudo-homogeneous model. The radial effective conductivity, λ_{er}, could be determined by fitting the temperature profiles predicted by the model with the experimental results as much as possible. Then, the ratio of radial effective conductivity to the conductivity of gas phase, λ_g, would be expressed as a function of the product between the pellet Reynolds number, Re_p, and the gas Prandtl number, Pr. For comparison, this method is also used to deal with the simulation results of the two metal structured packed beds, i.e. the simulated radial temperature profiles for the beds are considered as observed data to be fitted by the pseudo-homogeneous model to determine its effective heat transfer parameters. A series of values of λ_{er} can be obtained for specified structured packed bed and different operation conditions, and finally are correlated in terms of (λ_{er}/λ_g) versus ($RePr$), where Re is channel Reynolds number for the structured packed bed. Fig. 2 plots how the value of (λ_{er}/λ_g) changes with the value of ($RePr$) for the two metal structured packed beds, as well as the relationship between (λ_{er}/λ_g) and (Re_pPr) from the experimental pellet packed bed by Yang et al. [29].

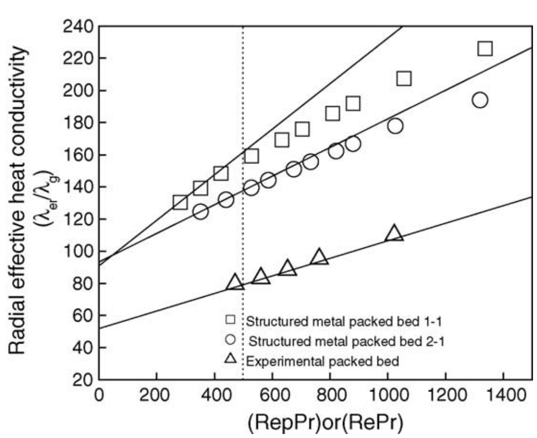

Fig. 2. The dimensionless radial effective conductivities of pellet and structured metal packed beds.

The dimensionless radial effective conductivity, (λ_{er}/λ_g), was linearly correlated with (Re_pPr), as shown in equation (8), for the experimental pellet packed bed considered here. However, for metal structured packed bed (λ_{er}/λ_g) cannot be correlated linearly with ($RePr$) except when ($RePr$) is less than 500. Equations (9) and (10) show the linear relationship between (λ_{er}/λ_g) and ($RePr$) when ($RePr$) is less than 500 for the metal structured packed bed 1–1 and 2–1, respectively.

$$\text{For pellet packed bed}: \quad \frac{\lambda_{er}}{\lambda_g} = 52.16 + 0.05638\,(Re_pPr) \tag{8}$$

For metal structured packed bed 1−1 :

$$\frac{\lambda_{er}}{\lambda_g} = 94.044 + 0.1284\,(RePr), \quad (RePr) < 500 \tag{9}$$

For metal structured packed bed 2−1 :

$$\frac{\lambda_{er}}{\lambda_g} = 94.841 + 0.0844\,(RePr), \quad (RePr) < 500 \tag{10}$$

In terms of the basic knowledge about effective heat transfer of conventional pellet packed bed, the first term in right side of these formulas denotes the contribution of static heat transfer such as conduction and radiation. The other term reflects the contribution of convection. It is found that the first terms in right side of equations (9) and (10) both are much more than that of equation (8). The reasons are probably as follows: heat resistance resulting from the contact of the pellets does not exist in the metal structured packed bed studied here and the conductivity of metal is much better than that of the pellets of γ-Al_2O_3. On the other hand, the voidage of the metal structured packed bed 2–1 is less than that of the bed 1–1, so the bed 2–1 has less conductive resistance which results in the larger first terms in right side of equation (10) than that of equation (9). Furthermore, the second term in right side of equation (9) is the most; the next is that of equation (10) and the least is that of equation (8). All these prove that the slope of the term on convection increases with the specific surface area of the bed.

Table 2
Necessary heights of different beds to reach the specified gas temperature

Object	Gas flux ($kg\ m^{-2}\ s^{-1}$)	Average temperature of gas at outlet of bed (°C)	Height of bed (m)
Pellet packed bed	3.78	369.10	0.742
Structured metal packed bed 1–1	3.79	369.12	0.450

3.1.2. The comparison in heat transfer ability and pressure drop

As shown in Table 1, the pellet packed bed has the same voidage of the bed and simulation conditions as the metal packed bed 1–1. To quantitatively validate the better heat transfer ability and hydrodynamic performance, the numerical simulation results for the metal structured packed bed 1–1 and the experimental data of the pellet packed bed are compared under the same operation conditions. The necessary heights of the two beds to reach the same gas temperature at the outlet are listed in Table 2.

It is found that, under the same flux, 3.78 $kg\ m^{-2}\ s^{-1}$, the metal structured packed bed 1–1 with height only 450 mm can achieve the same gas average temperature, 369.1 °C, as that of the pellet packed bed with height 742 mm. Fig. 3 shows the isolines of the temperatures in this bed in detail. Even if the height of the bed is less than 100 mm, gas temperature has been over 600 K and the excellent heat transfer performance of the metal structured packed bed is rather obvious.

Under the flux of 3.78 $kg\ m^{-2}\ s^{-1}$, using the well-known Ergun formula, the pressure drop of the pellet packed bed with height 0.45 m is calculated to be 33150.0 Pa. While the pressure drop of the metal structured packed bed 1–1 with height 0.45 m is calculated to be only 753.15 Pa. Fig. 4 shows the axial pressure profiles of the two kinds of beds.

It is clear that the pressure of the metal structured packed bed along the bed is almost invariable. Under this flux, the pressure drop of the pellet packed bed is about forty times as much as that of the metal structured packed bed.

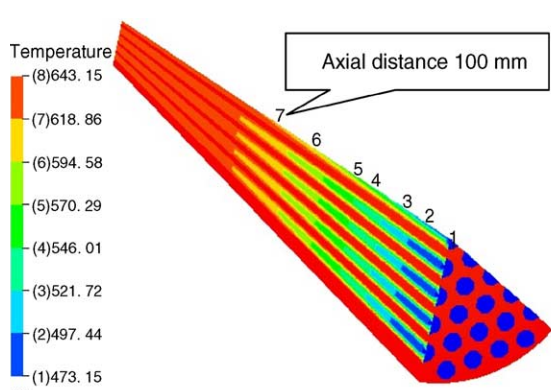

Fig. 3. The isolines of the temperatures in the structured metal packed bed 1–1.

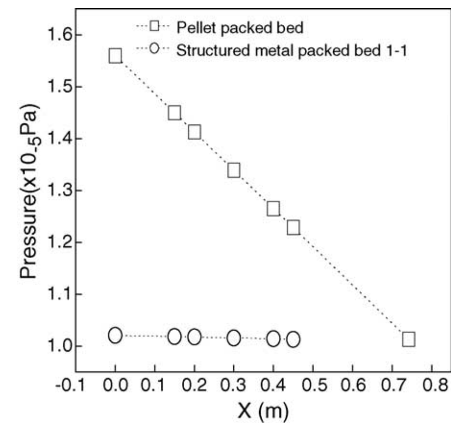

Fig. 4. The comparison of pressure profiles between pellet packed bed and structured metal packed bed 1–1.

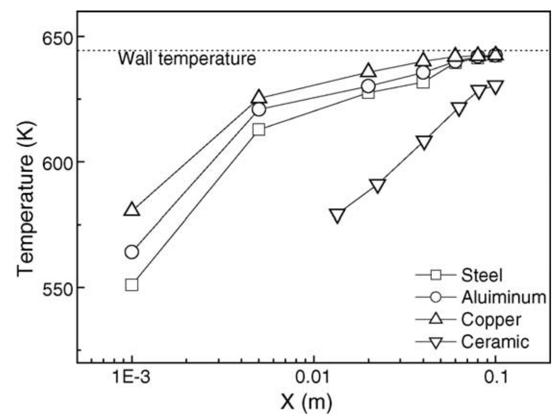

Fig. 5. The effect of structured material on heat transfer: $G = 0.76$ kg $m^{-2}\ s^{-1}$, $Re = 157.15$, $T_0 = 200$ °C and $T_w = 370$ °C.

3.2. The effect of the parameters on heat transfer performance

In this section, we discuss the effect of some parameters on the heat transfer performance of the metal structured packed bed.

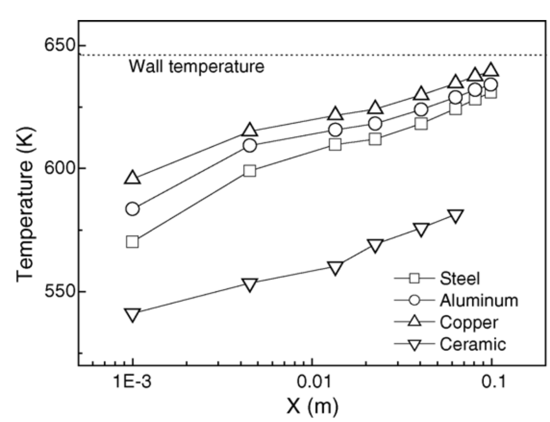

Fig. 6. The effect of structured material on heat transfer: $G = 4.38$ kg $m^{-2}\ s^{-1}$, $Re = 908.35$, $T_0 = 200$ °C and $T_w = 370$ °C.

Table 3
The structure parameters of simulated structured packed beds

Numbered bed	Height/diameter of bed (m/m)	Arrangement of channels	Number of channels (entries)	Aperture diameter (m)	Spacing of holes (mm)	Voidage of bed	Specific surface area (m^{-1})
Bed 2–1	0.5/0.035	Triangle	85	0.0020	~3.46	~0.28	55510
Bed 2–2	0.2/0.035	Triangle	85	~0.0026	~3.46	~0.45	72163
Bed 2–3	0.5/0.035	Triangle	55	0.0020	~4.04	~0.18	35918
Bed 2–4	0.2/0.035	Triangle	55	~0.0025	~4.04	~0.28	44897
Bed 2–5	0.2/0.035	Circle	85	0.0020	/	~0.28	55510

3.2.1. The effect of material property

The simulation is carried out for three kinds of metal structured packed beds consisting of different metal materials. The structure parameters and simulation conditions are the same as those of the metal structured packed bed 1–1 listed in Table 1. For two different gas fluxes, 0.76 and 4.38 kg m^{-2} s^{-1}, the axial profiles of gas average temperature over the three beds are shown in Figs. 5 and 6, respectively.

Note that the axial temperature profiles of the bed whose structured material is ceramic is added to Figs. 5 and 6 to validate the advantage of the metal structured packed bed over the non-metal structured packed bed. From these two figures, it is obvious that metal structured packed bed has much better heat transfer performance as we expected. The heat transfer ability of metal structured packed bed is so good that the change of gas temperature will be minor once the height of the bed is over 0.1 m, if chemical reaction does not take place as shown in Fig. 3. To consider the difference of the heat transfer, all figures are plot in the height less than 0.1 m. It can be seen that when *Re* is low, the effect of different materials on heat transfer is not apparent, but this effect became more evident when *Re* is larger.

3.2.2. The effect of the structure parameters

By means of changing the sizes, numbers and arrangement mode of the channels, five metal structured packed beds whose support material is aluminum with the different geometry parameters shown in Table 3, are designed. The simulation conditions are the same as those of metal structured packed bed 2–1 in Table 1. In the same way, for two different gas fluxes, 0.76 and 4.38 kg m^{-2} s^{-1}, the axial profiles of gas average temperature over the five beds are shown in Figs. 7 and 8.

From Fig. 7, it is found that when *Re* is low, the arrangement mode of the channels has little effect on heat transfer by comparing the beds 2–1 and 2–5, and it seems that the ability to transfer heat is proportional to the specific surface area of the bed by comparing the beds 2–1 and 2–4. However, from Fig. 8, it can be seen that when *Re* is high, the voidage of the bed began to determine the heat transfer performance because the skeletons of the five beds have the same property, and although the bed 2–2 has the largest specific surface area, its heat transfer performance is the poorest owing to the largest voidage. On the contrary, although the bed 2–3 has the smallest specific surface area, its heat transfer performance is the best because of the smallest voidage as seen in Fig. 8. It is possible that when *Re* is low, heat transfer is controlled by the convection. Therefore, the specific surface area determinates heat transfer at this time. When *Re* is high, heat transfer is controlled by the static contribution in this study, and the conduction strongly depends on the material property and the voidage of the bed. From Section 3.2.1, it has been known that the effect of the property of metal material gradually becomes important when *Re* is large, and it is consistent with the above analysis.

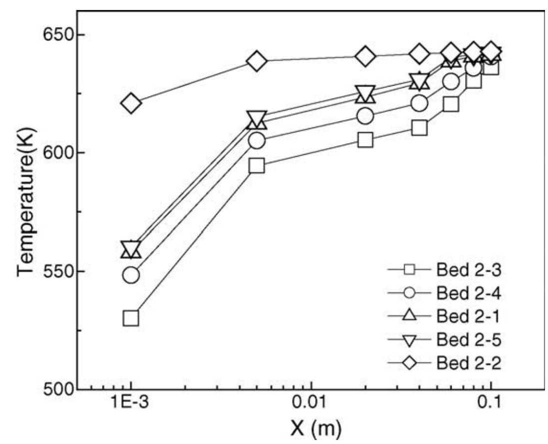

Fig. 7. The effects of structured parameters on heat transfer: $G = 0.76$ kg m^{-2} s^{-1}, $Re = 130.96–290.29$, $T_0 = 200$ °C and $T_w = 370$ °C.

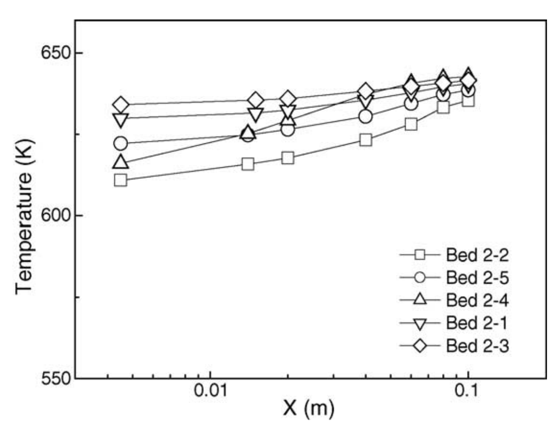

Fig. 8. The effects of structured parameters on heat transfer: $G = 4.38$ kg m^{-2} s^{-1}, $Re = 865.01–1684.41$, $T_0 = 200$ °C and $T_w = 370$ °C.

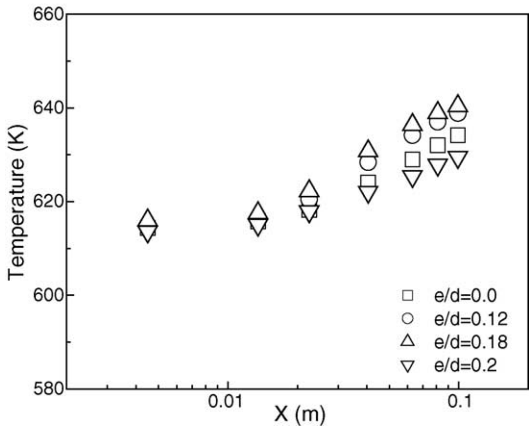

Fig. 9. The effect of the rough layer on heat transfer for larger *Re*.

3.3. The heat transfer enhancement of metal structured packed bed

According to the above results, at low *Re*, for the specified skeleton material and the voidage of the bed, it is obvious that increasing the specific surface area of the bed can intensify the heat transfer.

At high *Re*, the feasible method is to decrease the voidage or take advantage of materials with high intrinsic conductivity, but another method suggested here is to turn the smooth interface between the gas phase and solid phase into rough wall, and as we know, this way is only supposed to be valid for the turbulent flow. The bed 1–1 is used to verify this method. The structure parameters and simulation conditions are the same as that in Table 1. The gas flux adopted here is 4.38 kg m^{-2} s^{-1}. By choosing different height of rough layer, the temperature profiles predicted are shown in Fig. 9.

In Fig. 9, "*e*" refers to the average height of the rough layer at the interfaces and "*d*" refers to the diameter of the channel. As the increase of the value of "*e*", the gas average temperatures along the bed will go up. Actually, the effect will be more obvious when the gas flux is large enough to cause strong turbulence, which is not shown here. It can also be seen when the value of "*e*/*d*" exceeds 0.18, the temperature profile will run down instead. As a result of the analysis, it is important to decide the height of the rough layer for heat transfer enhancement at high *Re*. In this example, the best appropriate value of "*e*/*d*" is 0.18.

4. Summary and conclusions

Hydrodynamic and heat transfer performances of metal structured packed bed are simulated by using commercial software. For the metal structured packed bed studied here, the relationship between the effective heat transfer parameter (λ_{er}/λ_g) and the product of *Re* and *Pr* is non-linear, but when (*RePr*) is less than 500, it is approximately linear as that observed in the conventional pellet packed bed. In the relationship, the item that reflects the static heat transfer of the metal structured packed bed is much larger than that of the pellet packed bed. Moreover, the dependency of the convection contribution on Reynolds number is related to the specific surface area of the bed under the current conditions. Taking account of much larger specific surface area of metal structured packed bed than that of conventional pellet packed bed, it is more attractive to adopt structured metal as the support of catalyst.

Metal structured packed bed is quantitatively proved to have much better performance in heat transfer and much lower pressure drop in comparison with the conventional pellet packed bed. What is more, it has much advantage over the other non-metal structured packed beds.

By analyzing the effect of the parameters on heat transfer, it can be concluded that the heat transfer is controlled by the convection in low *Re* and increasing the specific surface area of the bed can effectively intensify it. But when *Re* is high, the static contribution dominates it. In this case, heat transfer can be improved by means of decreasing the voidage, mainly. Base on these results, some useful methods are proposed to enhance heat transfer. In particular, under turbulent flow, choosing an appropriate height of the rough layer is really helpful.

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