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RESEARCH PAPER

CFD Simulation of Porosity and Particle Diameter Influence on Wall-to-Bed Heat Transfer in Trickle Bed Reactors

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Abstract

Wall-to-bed (or wall-to-fluid) heat transfer issues in trickle bed reactors (TBR) has an important impact on operation and efficiency in this category of reactors. In this study, the hydrodynamic and thermal behavior of trickle bed reactors was simulated by means of computational fluid dynamics (CFD) technique. The multiphase behavior of trickle bed reactor was studied by the implementation of the Eulerian-Eulerian multiphase approach. Also, bed porosity effect was modeled by porosity function method. In order to study the effect of operating parameters on wall-to-bed heat transfer, the influence of catalyst particle diameter and catalytic bed porosity was investigated on wall-to-bed Nu number. The results showed that the enhancement of catalytic bed porosity from 0.36 to 0.5 decreases the Nu number about 15% due to a reduction of liquid velocity adjacent to the reactor wall. Also, the increase of particle diameter from 4 to 6 millimeter decreases wall-to-bed Nu number about 15% owing to a reduction in liquid phase volume fraction.

Keywords:
CFD Simulation,
Eulerian-Eulerian Approach,
Wall Effect,
Trickle Bed Reactors,
Wall-to-Bed Heat Transfer

Introduction

Fixed bed reactors are widely used in chemical, refinery, and petroleum industry. In this type of reactors, catalyst particles are held in place and do not move with respect to a fixed reference frame and the reaction of reactants occur by passing through the catalysts and generate the final product. A specific category of fixed bed reactors which are particularly used for the treatment of petroleum products in the refining industry and also for removing hazardous materials in the chemical industry are trickle bed reactors (TBR). In trickle bed reactors gas phase flow and liquid phase flow are co-current or counter-current, passing through the catalyst bed and it leads to exchange reactant components through phases and reaction on the catalyst surface. It is necessary to consider that the hydrodynamics of TBRs is a complex function of interactions of particle features, packing characteristics of the bed, features of gas and liquid, and operating conditions. In transport phenomena, particularly heat transfer two areas are explained in packed bed reactors: particles scale and bed scale. Heat transfer in particles scale can be easily described by the heat transfer coefficient for liquid-solid. In the case of TBR, particles are

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usually thought to be surrounded by a liquid film; however, this hypothesis should be corrected for low superficial liquid velocity for wetting of catalyst particles non-uniformly. One of the most significant instances about trickle bed reactors is to represent the geometric shape of the reactor according to the tens and hundreds of cylindrical reactors with a small ratio number of reactor diameter (D) to particle diameter (d) which is less than 10 (D/d_p) [1]. This is done to increase thermal exchange between substances in each cylindrical reactor with cooling fluid around it to better control operating conditions. Thus, study about the effect of operating parameters, wall-to-bed thermal exchange, and heat transfer are evaluated in variable types of operating conditions and have an important role in anticipating and designing trickle bed reactors. In many cases, the reactions carried out in TBRs are exothermic (e.g., hydrogenation, oxidation, and hydrotreating) so they liberated energy and also this energy poorly transfers in trickle bed reactors. Controlling this liberated energy without leading to unfavorable effects on the performance of TBRs like catalyst deactivation, is a vital task to successfully design and scale-up this type of reactors. There are different factors which affect the overall performance and heat transfer of TBRs like characteristics of catalytic bed (packing configuration, porosity, particle size) and operating conditions. There are different forms which heat transfer occurs in trickle bed reactors:

1. Heat transfer inside particles where reactions occur
2. Heat transfer from particles to fluid around catalyst particles
3. Heat transfer from particle to particle
4. Wall-to-bed heat transfer

Although, studies about trickle bed reactors are generally divided into two categories:

1. Wall-to-bed heat transfer in a single-phase flow
2. Two-phase flow wall-to-bed heat transfer

At first, an overview is presented about wall-to-fluid in the single-phase packed bed reactors. Miroliaei et al. [2] did research about the effect of operating conditions on wall heat transfer based on a CFD model. They applied an arrangement of catalyst particles in a computational domain and calculated wall-to-fluid heat transfer coefficient by passing the fluid over the particles in the CFD model. The comparison between simulation results and presented equations showed an accurate wall-fluid heat transfer anticipation of CFD model in references. Nijemeisland and Dixon [3] simulated a CFD model of wall-to-bed heat transfer in a fixed bed reactor. The case study of the catalyst bed included 44 particles and the amount of reactor-to-particle diameter ratio was 2. Results illustrated that numerical data satisfied reported data in references. Pang et al. [4] studied a fixed bed reactor with 3 various ratio numbers of the reactor to particle diameter. They investigated the local heat transfer coefficient of the wall. Consequences showed that the local heat transfer coefficient in the low range of reactor-to-bed particle diameter ratio has a fluctuating behavior.

Studies about wall-to-bed heat transfer in trickle bed reactors (including two liquid and gas phases) are discussed in the following part. In trickle bed reactors heat transfer coefficient between wall and fluid is related to fluid distribution around the wall and particularly depends on liquid phase properties [3]. The humidity of reactor walls oscillate and wall heat transfer rate is extremely related to velocity and liquid phase distribution around the wall in TBRs. Heat transfer between phases in fixed beds is a complex phenomenon that is described only by means of physical principles. That is why the mechanical model is presented in general:

$$Nu = \prod_{i=1}^{N} D_i^{b_i} \tag{1}$$

where D_i is a dimensionless number and b_i is their exponent, which is found by using experimental data. Presented equations for wall-to-fluid heat transfer has a general similarity with solid-to-fluid heat transfer. Muroyama et al. [5] considered dynamic liquid holdup as its primitive model for better prediction of heat transfer in the current conditions with strong interaction. They found that in trickle bed reactors, the wall-to-bed heat transfer rate is strongly related to liquid distribution and wall flow characteristics. Muroyama et al. [5] have suggested the following relationship between wall heat transfer to the liquid phase, using Reynolds and Prandtl numbers:

$$Nu = 0.012 Re_l^{1.7} Pr_l^{0.33} \quad (2)$$

Specchia et al. [6] also developed an equation for a weak interaction in TBRs similar to Muroyama et al. [5]. Mariyani et al. [7] worked on wall-to-bed heat transfer in the range of 4.7 to 34.3 bed-to-particle diameter ratio. They presented wall heat transfer coefficient as a reactor central core velocity function and based on Reynolds number and Prandtl number of the liquid phase, they showed that heat transfer value from the wall through inside of the trickle bed reactor is extremely related to liquid phase properties.

In the present research according to the importance of wall-to-bed heat transfer in trickle bed reactors efficiency and function, the impact of catalyst particle and bed porosity on the wall-to-bed thermal exchange will be studied in the form of dimensionless *Nu* number by means of a CFD model. It should be noted that *Nu*'s correlation has been created for a limited range of gas and liquid loads and for a specific catalyst shape and size. Therefore, there is a need for further research, including large-scale gas and liquid loads and different shapes and sizes of random packing, to better understand the heat transfer processes in complex geometric constraints.

Geometry of the Reactor and Boundary Conditions

Geometry and conditions of the examined reactor are presented in Fig. 1. Due to geometric symmetry and hydrodynamic in trickle bed reactors, it is possible to model the reactor hydrodynamic behavior accurately with the assistance of two-dimensional computational domains. Two-dimensional simulations of trickle bed reactors were presented in various papers such as [8-11] and the results showed the agreement of numerical and computational results. Hence in this article the two-dimensional model presented in Fig. 1 is applied to CFD simulation. Input boundary conditions in CFD model includes a two-phase of gas (air) and liquid (water) which enter respectively with a superficial velocity of 0.054 m/s and 0.0026 m/s from the top of the reactor. Inlet flow temperature and reactor wall temperature are respectively 310 and 300 °C.

Equations and Governing relations

Conservation Equations

In the present study, the Eulerian-Eulerian multiphase approach was applied to simulate multi-phase flow behavior. In this approach, the conservation equation of volume fraction, Eq. 1, and also momentum equation, Eq. 2, were presented for each phase. Conservation equations are expressed based on the following relations in Eulerian-Eulerian approach [11]:

$$\frac{\partial(\alpha_i \rho_i)}{\partial t} + \nabla.(\alpha_i \rho_i u_i) = S_i \quad (3)$$

$$\frac{\partial(\alpha_i\rho_i u_i)}{\partial t} + \nabla.(\alpha_i\rho_i {u_i}^2) = -\alpha_i\nabla P_i + \nabla.(\alpha_i\mu_i\nabla u_i) + \alpha_i\rho_i g + \sum_{i=1}^{n} F_{ji}(u_j - u_i) \quad (4)$$

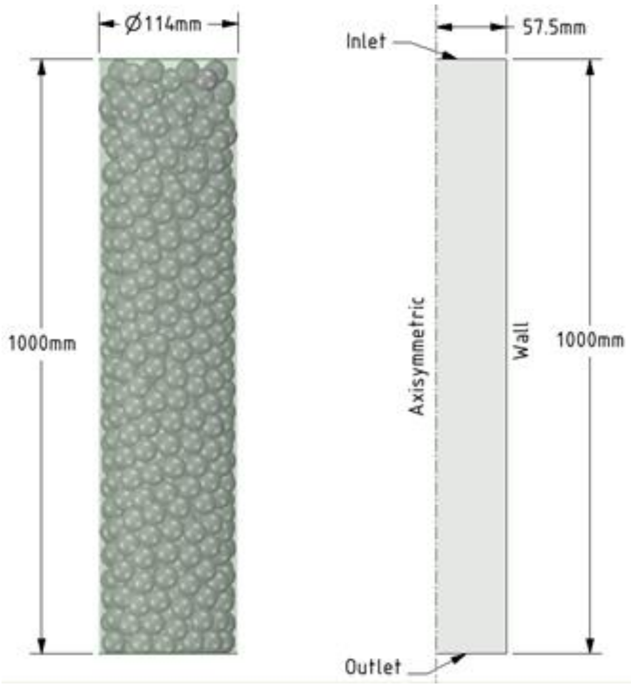

Fig. 1. Reactor geometry and two-dimensional computational domains with boundary conditions

where α_i, ρ_i, u_i and S_i are volume fraction, density, velocity, and source term in phase (i) (i can be gas or liquid phase). The most important expression which showed the interaction between phases in the multi-phase approach of Eulerian-Eulerian is F_{ji} in Eq. 2. This expression indicates the momentum interaction between phases j and i according to the concept of the drag coefficient. Regarding to this case, it is assumed that the surface of the catalysts is completely wetted buy the liquid, the term F_{ji} can represent F_{GL} and F_{LS}, which respectively indicate the interaction between phases (drag force) of gas-liquid and liquid-solid. F_{GL} and F_{LS} are presented by Attou et al. [12] as follows:

$$F_{GL} = \frac{\alpha_G}{\alpha_G + \alpha_L}\left(\frac{E_1\mu_G(1-\alpha_G)^2}{{\alpha_G}^2{d_p}^2} \times \left[\frac{\alpha_S}{(1-\alpha_G)}\right]^{0.667} + \frac{E_2\rho_G(u_G - u_L)(1-\alpha_G)}{{\alpha_G}^2{d_p}^2} \times \left[\frac{\alpha_S}{(1-\alpha_G)}\right]^{0.333}\right) \quad (5)$$

$$F_{LS} = \frac{1}{\alpha_G + \alpha_L}\left(\frac{E_1\mu_L(\alpha_S)^2}{{\alpha_L}^2{d_p}^2} + \frac{E_2\rho_L u_L(\alpha_S)}{\alpha_L d_p}\right) \quad (6)$$

In this case, the energy equation based on Eulerian approach is presented for each phase by the following relation:

$$\frac{\partial(\alpha_i\rho_i h_i)}{\partial t} + \nabla.(\alpha_i\rho_i u_i h_i) = \alpha_i\frac{\partial P_i}{\partial t} - \alpha_i\nabla(k_i.\nabla.T_i) + Q_{ij} \quad (7)$$

where Q_{ij} is interphase heat transfer and presented as:

$$Q_{ij} = h_{ij}A_{ij}(T_i - T_j) \quad (8)$$

where A is the thermal exchange surface and h is the heat transfer coefficient between phase i and phase j which can be calculated as follows:

$$h_{ij} = \frac{Nu_i k_j}{d_p} \tag{9}$$

where d_p is the particle diameter, k is the thermal conductivity coefficient and Nu is the Nusselt number that is calculated based on the following relation:

$$Nu_{ij} = 2 + Re_i^{1/2} Pr_i^{1/3} \tag{10}$$

where Re and Pr are respectively Reynolds number and Prandtl number for the ith phase.

Catalytic Bed Porosity Distribution

To illustrate the effect of porosity in catalytic bed reactors, two main approaches are used. In the first approach, the geometric arrangement of the catalyst particles is considered within the reactor; in the second method, the impact of solid phase presence is applied on the porosity distribution in the CFD model. The advantage of the first method is the high precision in describing the behavior of the reactor bed porosity, but it requires appropriate catalyst particles, fine meshing and therefore, high computational time. The second method is also accurate in the modeling of the bed porosity behavior and in the opposite way, it does not have the problem of creating a fine mesh and also the catalyst particle arrangement. Considering that the second method is one of the most widely used methods for simulating the effect of porous media in trickle bed reactors, for example, references [8,9,11,13], in this study, the second method was also used to express the effect of the porous medium. For spherical particles, the porosity distribution relation is given as follows [10]:

$$\epsilon(r) = \epsilon_b + (1 - \epsilon_b) J_0(a \times r^*) e^{-b \times r^*} \tag{11}$$

If $2.61 \leq D/d_p \leq 13.0$:

$$a = 8.243 - \frac{12.98}{\left(D/d_p + 3.156\right)} \tag{12}$$

If $2.61\, D/d_p > 13.0$:

$$a = 7.383 - \frac{2.932}{\left(D/d_p - 9.864\right)} \tag{13}$$

$$b = 0.304 - \frac{0.724}{D/d_p} \tag{14}$$

$$r^* = \frac{R - r}{d_p} \tag{15}$$

In Eq. 13, J_0 is the zero order Bessel function, ϵ_b is the bed medium porosity and r is the radial distance from the bed axis.

Table 1. Case study

Conditions	Particle diameter(mm)	Bed porosity
Case-1	0.003	0.36
Case-2	0.003	0.40
Case-3	0.003	0.45
Case-4	0.003	0.50
Case-5	0.004	0.36
Case-6	0.005	0.36
Case-7	0.006	0.36

Results

Reviewed Operating Conditions

In order to investigate the effect of porosity and particle diameter on the amount of wall-to-bed heat transfer in the trickle bed reactor, 7 different types of operating conditions were studied. Table 1 represents the operating conditions. Nusselt number is presented in the final results to calculate the effect of operating parameters (particle diameter and bed porosity) on the amount of wall-to-fluid heat transfer. Wall-to-fluid *Nu* number based on liquid-phase properties is given as follows:

$$Nu = \frac{hd_p}{k_L} \quad (16)$$

where k_L is the thermal conductivity coefficient and h is the heat transfer coefficient which is calculated as follows:

$$h = \frac{\dot{m}_{out}H_{out} - \dot{m}_{in}H_{in}}{A(T_{out} - T_{in})} \quad (17)$$

where H is the enthalpy and $\dot{m}$ is the mass flow rate, the *out* index and the *in* index represent output and input of the reactor.

Governing equations were solved by the finite volume method. To solve the pressure-velocity field problem, the SIMPLE (Semi-implicit method for pressure linked equations) method was used and QUICK (quadratic upwind interpolation for convective kinematics) method was applied to discretize the momentum and continuity equations.

Mesh Independency

To investigate meshing independency three different mesh sizes were studied with the mesh sizes of 14500 (mesh1), 88720 (mesh 2) and 355000 (mesh3) in the CFD model to evaluate TBR pressure drop. Among the three types of examined mesh, the difference between the predicted pressure drop was less than 0.1% between the second and third meshes. Considering that the second type has fewer nodes than the third mesh and also its computational time is lower than the third mesh, the second mesh was applied for calculation in this study.

Porosity Effect on the Wall-To-Bed Heat Transfer

The impact of the bed porosity on the wall-fluid heat transfer based on case-1 to case-4 (Table 1) conditions in trickle bed reactors were illustrated in Fig. 2. As shown in this figure, by increasing the particle diameter, the Nu number of the wall or, in other words, the amount of heat exchange between the wall and fluid was decreased. Fig. 3 illustrates the radial temperature variation in different porosities of the catalytic bed in the middle of the reactor. The results indicate an intense change in temperature profiles near the wall. At adjacent to the wall, gas and liquid phases flow with more velocity due to the low drag resistance of the fluids with particles (wall effect). Therefore, high heat exchange between fluid and wall occurs near the wall, and temperature profile decreases immediately at the wall region.

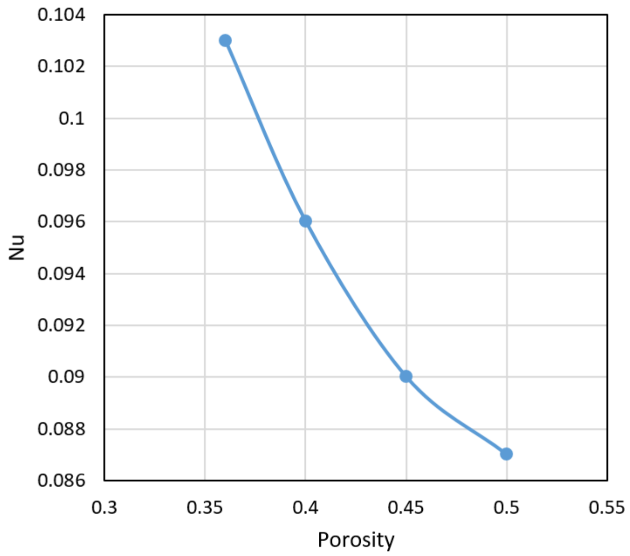

Fig. 2. Bed porosity effect on the Nu number of the wall-fluid

In order to determine the effect of the particle diameter on the *Nu* number, the average fluid velocity was presented up to 3mm from the wall in Fig. 4. As illustrated in this figure, with increasing the bed porosity, the amount of liquid phase velocity adjacent to the wall decreased and More space was created to pass through the phases inside the reactor bed by increasing the bed porosity. Therefore, the liquid phase velocity decreased with increasing the bed porosity. Considering that the examined liquid phase, is water fluid and gas phase is an air-fluid and the thermal conductivity coefficient of the liquid phase is 25 times the gas phase, thus the liquid phase plays a decisive role in the heat exchange of the wall-fluid. According to that, the liquid phase velocity decreased along the wall by increasing the porosity, the heat exchange rate of the wall-fluid, which is a function of the phases velocity and its thermal conductivity, also showed a decreasing behavior (Fig. 2).

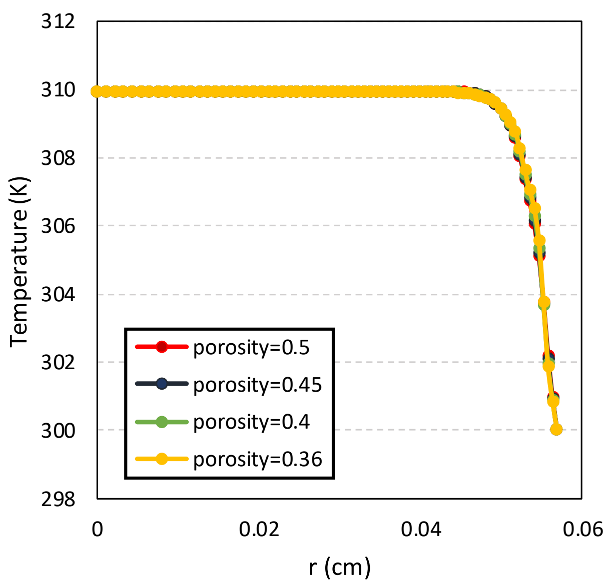

Fig. 3. Temperature variation process in different porosities

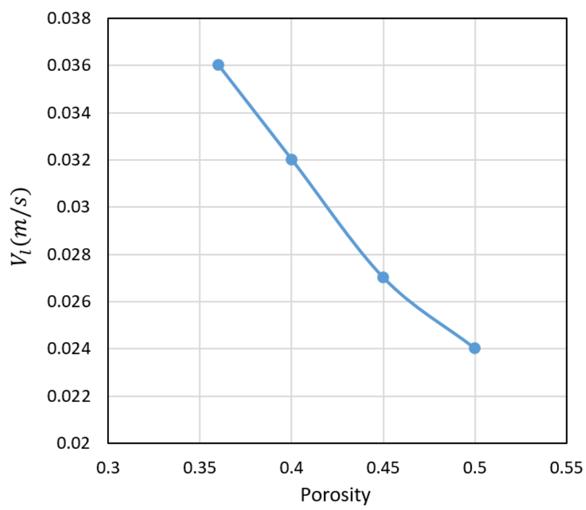

Fig. 4. The effect of bed porosity on the liquid phase velocity adjacent to the wall

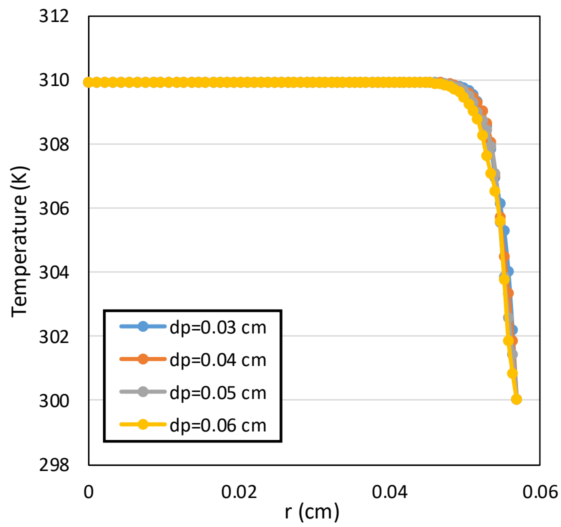

Fig. 5. Comparison of temperature variations in different diameters

Particle Diameter Effect on the Wall-To- Bed Heat Transfer

Fig. 5 shows the temperature variations in different particle sizes through the reactor diameter, which shows more changes in the fluid temperature than porosity variations in the reactor. These results indicate that, by decreasing the volume fraction of the liquid due to the increase of packing's diameter around the wall of the reactor (Fig. 6), the liquid temperature also changes to some extent.

In Fig. 7 particle diameter impact was shown on the *Nu* number of the wall based on case-5 to case-7 conditions of Table 1. As shown in this figure with an increasing particle inside of the bed, the *Nu* number of the wall decreased. To investigate the particle diameter effect on Nu number, the impact of particle diameter was examined on the volume fraction of the liquid phase adjacent to the wall (Fig. 6). According to Fig. 6 with increasing of the particle diameter, the volume fraction of the liquid phase along the wall showed a decreasing procedure. Due to the higher thermal conductivity of liquid phase in comparison to the gas (air) phase, by decreasing the volume fraction of the liquid phase along the wall, considering that the liquid phase (water) plays a very important role in the wall-to-bed thermal exchange, the amount of thermal exchange of the wall-fluid decreased. As a result, by increasing the catalyst particles diameter, wall-to-bed heat transfer coefficient and wall-fluid Nu number had a decreasing procedure.

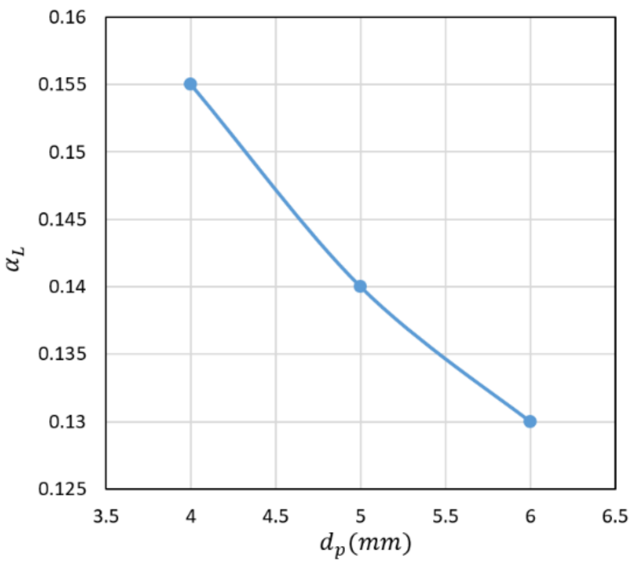

Fig. 6. Particles diameter effect on the volume fraction of the liquid phase along the wall

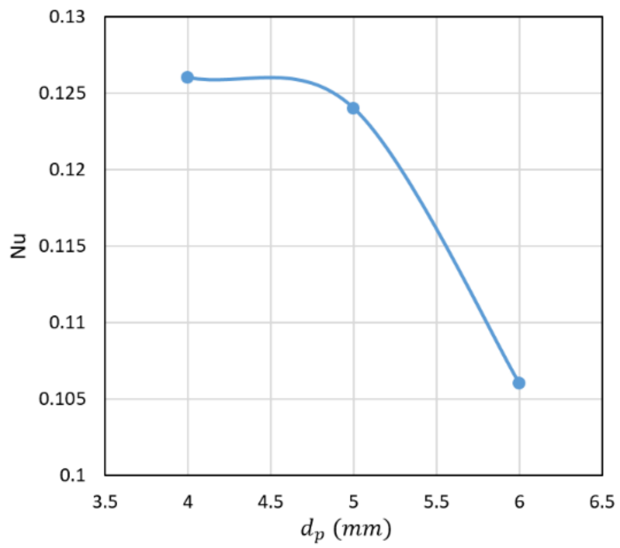

Fig. 7. The effect of particles diameter on the wall-to-bed Nu number

Conclusions

In this article, the effect of the bed porosity and catalyst particles diameter were studied on wall-to-bed heat transfer in trickle bed reactors by means of Eulerian-Eulerian approach and using porosity distribution function. Given the fact that study of the thermal behavior in trickle bed reactors is a function of the reactor's hydrodynamics behavior, first, a suitable model was developed to predict the reactor's hydrodynamics behavior. After presenting the hydrodynamics model, by examining the effect of bed porosity and particles diameter on the wall-to-bed heat transfer, wall-to-bed Nu number at different operational conditions was evaluated. The results showed that, by increasing the porosity of the catalytic bed due to the decrease of the liquid phase velocity along the wall, the wall-to-bed Nu number reduces by increasing bed porosity. Also, the study of the diameters of the particles illustrated that the amount of the liquid phase volume fraction decreased along the wall with increasing particles diameter of the catalytic bed. The reduction of the liquid phase volume fraction along the wall also showed the effect of reducing the exchange of the wall-to-bed heat transfer in the reactor and reduction in the wall-to-bed Nu number.

Nomenclature

A Thermal exchange surface (m^3)
d_p Particle diameter (m)
D Bed diameter (m)
h Heat transfer coefficient ($wm^{-2}k^{-1}$)
H Enthalpy ($Pa.m^3$)
J_0 Bessel function of first kind, order zero
k_l Thermal conductivity coefficient ($w.m^{-1}k^{-1}$)
$\dot{m}$ Mass flow rate (kgs^{-1})
N Bed particle diameter ratio
Nu Nusselt number
Pr Prandtl number
r Radial diameter from the center of the bed (m)
Re Reynolds number
s Source term (J)
u Velocity (ms^{-1})

Greek letters
α Volume fraction
ε Bed void fraction
μ Dynamic viscosity ($Pa\ s$)
ρ Density (kgm^{-3})

Subscripts
G Gas
L Liquid
r Radial
S Solid

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