CFD simulation of wall to fluid heat transfer coefficient in trickle bed reactors with cylindrical trilobe packing

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Abstract
Heat transfer issue in trickle bed reactors is one of the notable problem in chemical engineering. A trickle bed reactor is a type of fixed bed reactor, in which the two phases of gas and liquid pass through the catalytic bed in contact with each other and are used in a variety of industries including petrochemicals. In this study, we investigate the effect of Reynolds number changes on wall to fluid heat transfer in trickle bed reactors using CFD method. This reactor consists of cylindrical packs that are randomly placed inside the reactor. As the liquid Reynolds number increases, significant changes are observed in the wall to fluid Nusselt number. However, with increasing the Reynolds number of gas phase and keeping the Reynolds number of liquid phase constant, no significant changes in the wall-fluid Nusselt number could be observed.

Keywords: Trickle bed reactors, CFD simulation, Eulerian-Eulerian approach, wall-to-fluid heat transfer

Introduction
One of the type of fixed bed reactor which is widely used as a multiphase catalytic reactor is a trickle bed reactor. These reactors have a non-moving bed with catalytic particles and the liquid and gas phases flow over these particles. Trickle bed reactors are used in the petroleum, petrochemical, chemical, biochemical, electrochemical and wastewater treatment industries. These types of reactors have advantages in terms of cost and simplicity, but understanding the complex hydrodynamics inside these multi-phase (gas-liquid-solid) reactors is very challenging [1]. The complexity of the fluid dynamics behavior causes uncertainty to calculate the transport parameters in the reactor modeling, with heat transfer parameters playing an important role in the design of catalytic reactors [2]. Therefore, proper investigation of the fluid dynamic behavior inside the reactor is essential for the calculation of heat transfer parameters. With advances in computer performance and advances in numerical techniques and algorithms, the use of computational fluid dynamics (CFD) simulations has greatly increased in designing reactors as an efficient method for the complex hydrodynamics calculation of these reactors. The computer produces either random or non-random catalytic particles and the meshing strategies are intensely investigated, especially the behavior of the contact points to prevent cell skewness and increase convergence (Dixon et al.) [3] CFD simulation has become a very useful tool for chemical engineers to better understand the reactor hydrodynamics and the design and

development of a variety of fixed bed reactors. The process of heat transfer is very important in both cases, operation and safety. Most chemical reactions are either exothermic or endothermic, so to keep the process safe in the reactor, the temperature must always be kept at an appropriate temperature. Areas of studying wall-to-fluid heat transfer in fixed bed reactors include two parts. The first part deals with studies of wall-to-fluid heat transfer in single-phase flow within the reactor and the second part deals with wall-to-fluid heat transfer in two-phase flow within the reactor (trickle bed reactor). In the following part, we point out to some studies of wall-to-fluid heat transfer in single phase flow. In 2001 N.J.Mariania et al. [4] investigated the parameters of heat transfer in a fixed bed with a downward gas-liquid flow. Experimental investigations of heat transfer in fixed bed reactors using 2DPPF (two dimensional pseudo-homogeneous plug flow) model and obtaining equations based on experimental results for wall heat transfer coefficient (h_w) and effective thermal conductivity (k_{er}) showed that The model is inappropriate for the low bed to particle diameter aspect ratio. Michiel Nijemeisland, Anthony G. Dixon [5] studied CFD simulation of wall heat transfer and fluid flow in a fixed bed reactor filled with spherical packing. Investigation of the relationship between local flow field and local wall heat flux showed that local heat transfer rates were not statistically correlated with local flow field. Local patterns of wall heat flux are related to larger-scale flow structures in the bed. In 2004 A.Guardo et al. [6] studied the effect of turbulent model on CFD modeling of wall-to-bed heat transfer in fixed bed reactors for different RANS models (Spalarat-Allmaras, k-ω, k-ε). As a result of this study, the Spalarat-Allmaras model outperformed the other two RANS models for predicting pressure drop and heat transfer. In 2003, NéstorJ.Mariani et al. [7] investigated the effect of liquid radial distribution on heat transfer parameters as well as the ratio of column to particle diameter on radial heat transfer in trickle bed reactors. Finally, equations for effective radial thermal conductivity in the central region (ker,c) and the heat transfer coefficient of the wall region to the wall tube (hw,c) were developed. Amir heidari et al. [8] developed micro-scale and meso-scale models to investigate the heat transfer between gas and liquid phases. The results showed that with increasing the gas phase Reynolds and Prandtel number the Nusselt number increased, also with increasing the gas phase Reynolds and the liquid phase Prandtel and Eö number the Nusselt number decreased. In this study, a new equation for the gas-liquid interfacial Nusselt number is presented for micro and meso scale reactors. Maria J. Taulamet et al. [9] studied the influence of particle shape and size as well as operating conditions on the prediction of thermal behavior of the trickle bed reactor. The results of this study were presented to predict equations for h_w and k_{er} for different particle shape and size and also for different operating conditions.

Boundary conditions and reactor geometry

The geometry and boundary conditions of the reactor are presented in Fig. (1). According to the geometrical symmetry and the hydrodynamic of the trickle bed reactor, the computational domain can be considered less than the whole domain, for the purpose of faster computation. Therefore, in this study one eighth of the reactor was considered as the computational domain. Packing particles with a diameter of 2.6 mm are randomly placed in the reactor. These particles are randomly arranged in the reactor using Algoryx Momentum. Algoryx Momentum is about developing, validating and visualizing the performance of mechanical systems. It is also used to convert dynamic simulations into CAD (computer-aided design) models [10]. The length of the reactor is 270 mm and its diameter is 51.4 mm. The inlet to the reactor consists of two phases of gas (air) and liquid (water) that flow into the reactor. The inlet flow temperature to the reactor is 90 ° C and the wall temperature is 80 ° C.

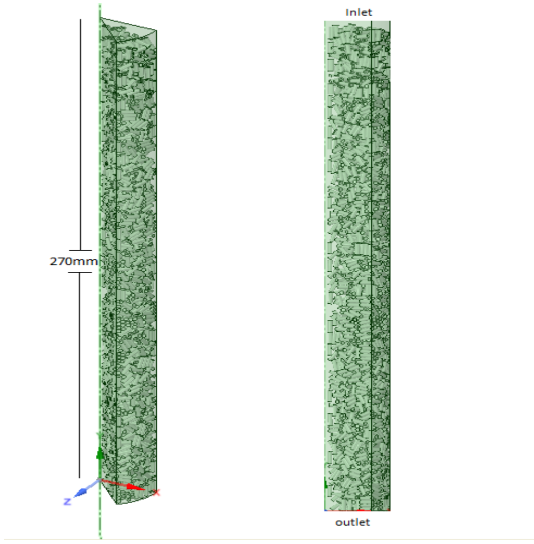

Fig 1. The geometry of the trickle bed reactor

Governing Equations

Conservation equations

In this study the Eulerian-Eulerian approach was used to investigate the multi-phase flow behavior. In the Eulerian-Eulerian model, the volume fraction conservation equation (1) and the momentum equation (2) are presented for each phase. The conservation equations in the Eulerian-Eulerian approach are stated below [11]:

$$\frac{\partial(\alpha_i \rho_i)}{\partial t} + \nabla.(\alpha_i \rho_i u_i) = S_i \tag{1}$$

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

In these equations α_i ،ρ_i ،u_i and $S_i$are respectively the volume fraction, density, velocity, and production and consumption terms in phase i ("i" refers to the gas, liquid, and solid phases). The most important expression in the multi-phase Eulerian approach that shows the interaction between phases, is F_{ji} in Equation (3). These expressions state that, the momentum interaction between phase j and i is based on the concept of drag coefficient. The term F_{ji} can denote F_{GL} and F_{LS}, which represent the gas-liquid and liquid-solid phase interactions, respectively. F_{GL} and F_{LS} were presented by Attou et al. [12] as follows:

$$F_{GL} = \frac{\alpha_G}{\alpha_G + \alpha_L}\left(\frac{E_1 \mu_G (1-\alpha_G)^2}{{\alpha_G}^2 {d_p}^2}\left[\frac{\alpha_S}{(1-\alpha_G)}\right]^{0.667} + \frac{E_2 \rho_G (u_G - u_L)(1-\alpha_G)}{{\alpha_G}^2 {d_p}^2}\left[\frac{\alpha_S}{(1-\alpha_G)}\right]^{0.333}\right) \tag{3}$$

$$F_{LS} = \frac{1}{\alpha_G + \alpha_L}\left(\frac{E_1 \mu_L (\alpha_S)^2}{{\alpha_L}^2 {d_p}^2} + \frac{E_2 \rho_L u_L (\alpha_S)}{\alpha_L d_p}\right) \tag{4}$$

In this study, due to considering the heat transfer, the energy equation is investigated in the Eulerian-Eulerian approach. The following energy equation for each phase is as follows:

$$\frac{\partial(\alpha_i\rho_i h_i)}{\partial t} + \nabla.(\alpha_i\rho_i u_i h_i) = \alpha_i\frac{\partial P_i}{\partial t} - \alpha_i\nabla(k_i.\nabla.T_i) + Q_{ij} \quad (5)$$

In the above equation h, T, k, and Q_{ij} are enthalpy, temperature, thermal conductivity and heat transfer rate between phase i and j respectively. In order to calculate the rate of heat transfer between phase i and j, the term Q_{ij} is showed in Equation (6):

$$Q_{ij} = h_{ij}A_{ij}(T_i - T_j) \quad (6)$$

Where A and h are the heat exchange area and the heat transfer coefficient between phase i and j, which can be calculated as follows:

$$h_{ij} = \frac{Nu_i k_j}{d_p} \quad (7)$$

Where d_p is the particle diameter, k is the thermal conductivity and Nu is the Nusselt number.

Study of operating conditions

In this work, it is worth mentioning that Ansys Fluent V.18.0 software was used to solve the equations. SIMPLE method was used to solve the pressure-velocity field in the problem and the First Order Upwind method was used to discrete the momentum equations. In order to investigate the effect of the gas and liquid phases Reynolds number on the wall to bed heat transfer in a trickle bed reactor containing cylindrical packing, different operating conditions have been investigated. In Table (1), eight different operating conditions that were examined are illustrated. To calculate the effect of different operating conditions (Reynolds number variations) on wall to bed heat transfer, we used non dimensional Nusselt number and compare these numbers with the results obtained. The Nusselt number equation based on the liquid phase is given below:

$$Nu = \frac{hd_p}{k_L} \quad (8)$$

In the above equation k_L is the thermal conductivity of the liquid phase and h is the heat transfer coefficient which is calculated based on the following equation:

$$h = \frac{\dot{m}_{out}H_{out} - \dot{m}_{in}H_{in}}{A(T_{out} - T_{in})} \quad (9)$$

Where H and m represent the enthalpy and the mass flow rate. The index in and out, respectively, represent the reactor inlet and outlet.

Table 1. Operating Conditions

Case	Re_L	Re_G
Case-1	13.02	18
Case-2	30.1667	18
Case-3	37.56	18
Case-4	45.58	18

Case-5	13.02	15
Case-6	13.02	21
Case-7	13.02	30
Case-8	13.02	50

Study of the mesh independency

To investigate the mesh independency three different approaches for predicting the Nusselt number were examined. Finally, the mesh with 285,000 nodes is used in comparison to the other two meshes due to its more accurate Nusselt number prediction.

Validation

Experimental data for the Nusselt number were extracted from Taulamet et al. [9] and compared with CFD data obtained in this study. The CFD method with an error of 10.3% compared to the experimental data in the present paper was used for this study.

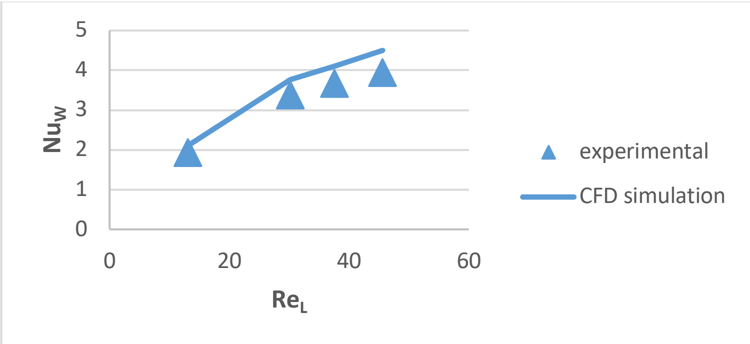

Fig 2. experimental data for cylindrical packing with an equivalent diameter of 2.6 for different operating conditions are shown using blue triangles.

Table 2. shows the percentage of error obtained by comparing the wall to bed Nusselt numbers from experimental method to the CFD simulation.

Table 2. Error percentage analysis of experimental data with CFD modeling

Re_L	Nu_{wall}(experimental)	Nu_{wall}(CFD simulation)	Error (%)
13.02	1.93	2.1	0.081
30.167	3.38	3.76	0.101
37.56	3.66	4.1	0.107
45.58	3.94	4.5	0.1244

Results and discussion

Investigation of the effect of Reynolds number changes on liquid and gas phases Figure 3. shows the effect of Reynolds number changes on the wall to bed Nusselt number for Case-1 to Case-4 operating conditions. In this case, we consider the Reynolds number of the gas phase constant and calculate the wall Nusselt number in different liquid phase Reynolds numbers.

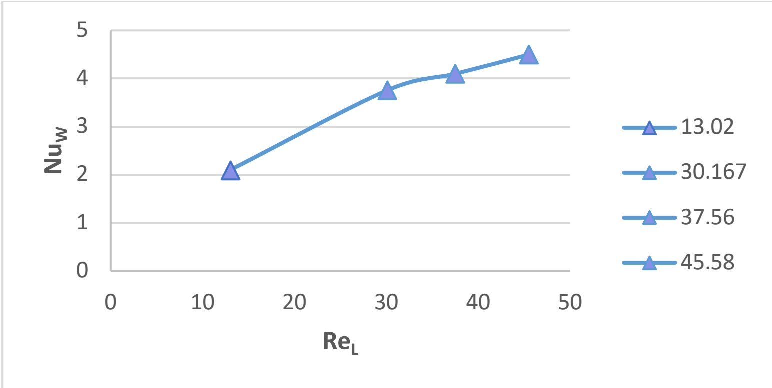

Fig 3. The effect of liquid phase Reynolds number on the Nusselt of the wall

Fig 4. also shows the effect of Reynolds number of gas phase under Case-5 to Case-8 on wall to bed Nusselt number. In this section, we consider the Reynolds number of the liquid phase constant and assume the gas phase Reynolds number as a variable, to investigate the effect of these conditions on the Nusselt number of the wall.

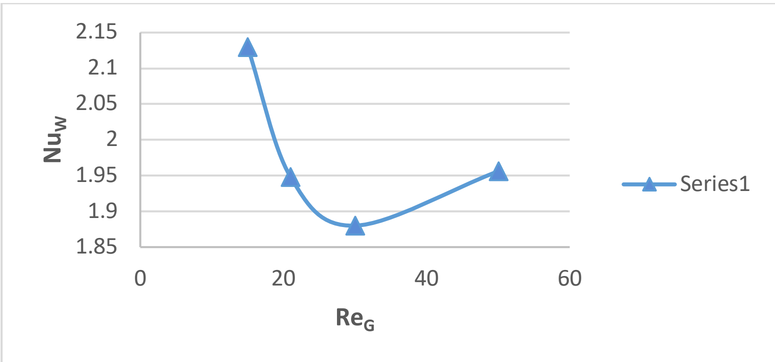

Fig 4. Influence of gas phase Reynolds number changes on the Nusselt of the wall

As shown in Figure 5. with the gas phase Reynolds number changes, there is no significant change in the wall Nusselt number. However, these changes are observable with increasing the liquid phase Reynolds number.

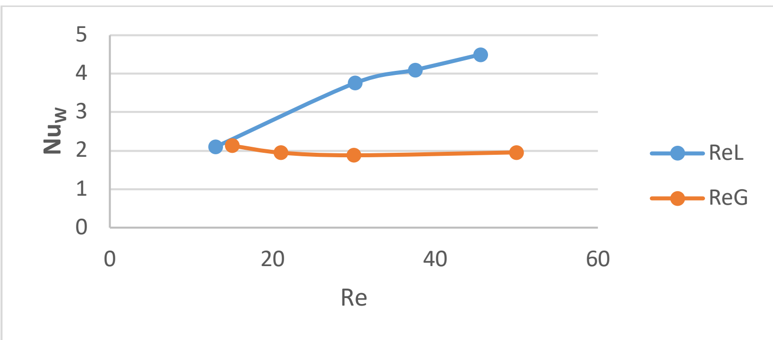

Fig 5. Comparison of the effect of Reynolds gas and liquid phase changes on the Nusselt number of the wall

Conclusions

In this paper, the effect of the gas and liquid Reynolds number on wall to bed heat transfer in a trickle bed reactor was investigated using a multi-phase Eulerian-Eulerian approach. Since the study of thermal behavior in trickle bed reactors is a function of the hydrodynamic behavior of the reactor, it was first modeled by developing an appropriate model of the phase interaction in the reactor. After presenting the hydrodynamic model, by investigating the effect of the gas and liquid phases Reynolds number on wall to bed heat transfer, their effect on wall to bed Nusselt number was presented. The results with respect to the effect of Reynolds number on the Nusselt number of the wall showed that the gas phase velocity changes at the inlet of the reactor had little effect on the wall to bed heat transfer. However, it demonstrated that the liquid phase velocity changes at the inlet of the reactor had a noticeable effect on wall to bed heat transfer in the trickle bed reactor.

References

[1] WU Qiang, 2004. Wastewater treatment by catalytic wet air oxidation in a continuous pilot-scale trickle bed reactor, February

[2] Dafydd Daviesa, Stanislaw Golunskia, Peter Johnston ,2018. Dominant effect of support wettability on the reaction pathway for Catalytic Wet Air Oxidation over Pt and Ru nano-particle catalysts, Catalysis, February 22

[3] Anthony G. Dixon,2012. Experimental validation of high Reynolds number CFD simulations of heat transfer in a pilot-scale fixed bed tube, Chemical Engineering Journal 200–202 (2012) 344–356

[4] N.J. Mariania, O.M. Martínezac, F. Barretoa,2001. Evaluation of heat transfer parameters in packed beds with cocurrent downflow of liquid and gas, Chemical Engineering Science, Volume 56, Issues 21–22, November 2001, Pages 5995-6001.

[5] Michiel Nijemeisland and Anthony G. Dixon,2004. CFD Study of Fluid Flow and Wall Heat Transfer in a Fixed Bed of Spheres, AIChE J, 50: 906–921.

[6] A. Guardoa,, M. Coussiratb, M.A. Larrayoza, F. Recasensa, E. Egusquizab,2004. Influence of the turbulence model in CFD modeling of wall-to-fluid heat transfer in packed beds, Chemical Engineering Science 60 (2005) 1733–1742.

[7] Mariani, N.J., Mazza, G.D., Martínez, O.M., Cukierman, A.L., Barreto, G.F., 2003. "On the influence of liquid distribution on heat transfer parameters in trickle bed systems", *Can J Chem Eng*, 81(3-4), pp. 814-820.

[8] Amir Heidari, 2013.Numerical evaluation of the gas–liquid interfacial heat transfers in the trickle flow regime of packed beds at the micro and meso-scale, Chemical EngineeringScience104(2013)674–689

[9] María J. Taulamet,2017, Prediction of thermal behavior of trickle bed reactors: The effect of the pellet shape and size, Fuel, Volume 202, Pages 631-640.

[10]Algoryx, Algoryx Momentum, visited on 2017-12-12. [Online]. Available: https://www.algoryx.se/mainpage/wp-content/uploads/2017/03/Algoryx-Momentum-DataSheet.pdf.

[11] Gunjal, P.R., Ranade, V.V., 2007. "Modeling of laboratory and commercial scale hydro-processing reactors using CFD", *Chemical Engineering Science*, 62(18), September, pp. 5512-5526.

[12] Attou, A., Ferschneider, G., 1999. "A two-fluid model for flow regime transition in gas-liquid trickle-bed reactors", *Chemical Engineering Science*, 54(21), pp. 5031-5037.