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Numerical evaluation of the gas–liquid interfacial heat transfer in the trickle flow regime of packed beds at the micro and meso-scale

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HIGHLIGHTS

- Interfacial heat transfer has been investigated in the micro and meso-scale structure of the trickle bed reactor.
- Effects of the gas and liquid Reynolds and Prandtl numbers and also Eötvös number have been studied on the interfacial Nusselt number.
- A new correlation has been developed to evaluate interfacial Nusselt number in the micro-scale.

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ABSTRACT

In the present work, two different models (micro-scale and meso-scale) were developed to investigate the heat transfer between the gas and liquid phases in the trickle flow regime of a packed bed reactor. In the micro-scale model, a simplified description of bed geometry, known as the double-slit model, was implemented to study the effects of different operating parameters, in terms of gas and liquid Reynolds, Prandtl and Eötvös numbers, on the interfacial Nusselt number. In the meso-scale model, the Volume-of-Fluid (VOF) approach was used to simulate trilobe, cylindrical and spherical catalyst shapes and accurately predict the effects of interface morphology and bed geometry on interfacial heat transfer. To validate the implemented methods, a simple packed bed reactor with spherical catalysts was developed to experimentally investigate the interfacial heat transfer of co-current, downward gas–liquid film flows. The results obtained from CFD simulations and experimental data were in agreement and accurately predicted bed reactor temperature profiles with a mean relative error of 2.15%. In both the micro- and meso-scale models, an increase in the Reynolds and Prandtl numbers increased the interfacial Nusselt number; whereas, an increase in dimensionless groups of the liquid phase or the Eötvös number caused the opposite effect. Finally, a new correlation was proposed that evaluated the gas–liquid Nusselt number in the trickle flow regime with a standard deviation of 7.19% compared to results acquired using the micro-scale model.

1. Introduction

Trickle bed reactors (TBR) are a group of highly efficient catalytic packed bed reactors that are widely used in chemical and petrochemical industries, such as in petroleum refineries, for hydrotreatment, hydrofinishing, hydrodesulfurization and hydrocracking applications (Bhaskar et al., 2004). In most TBRs, the gas and liquid phases flow co-currently through catalytic beds that have a different porosity and catalyst shape in the trickle flow regime (Ranade et al., 2011). In this regime, the liquid film wets the catalyst surface so the gas phase can flow continuously between the wetted catalysts. Therefore, the hydrodynamics of the packed bed is a critical parameter in the development of appropriate models that describe the interfacial phenomena of TBRs, such as mass and heat transfer.

Over the past few decades, numerous experimental and numerical simulations have been performed that evaluate the effect of catalytic bed structure, flow pattern and operating condition on the hydrodynamic properties of TBRs (Wang et al., 2013). Previous experimental studies have investigated many hydrodynamic properties of TBRs while varying catalyst geometry and operating conditions, such as pressure drop (Salimi et al., 2013; Aydin and Larachi, 2005; Bazmi et al., 2011a; Boyer et al., 2007; Calis et al., 2001; Freund et al., 2003; Gunjal and Ranade, 2007; Gunjal et al., 2003; Iliuta and Larachi, 2002; Lakota et al., 2002; Macías and Ancheyta, 2004; Nemec and Levec, 2005), maldistribution (Atta et al., 2007a; Bazmi et al., 2012; Crine et al., 1992; Funk et al., 1990; Gunjal and Ranade, 2007; Hanratty and Duduković, 1992; Jiang et al., 2001, 1999; Llamas et al., 2008; Lopes and Quinta-Ferreira, 2009; McManus et al., 1993; Schubert et al., 2008), liquid holdup (Aydin and Larachi, 2005; Bazmi et al., 2011a; Boyer et al., 2007; Gunjal et al., 2005; Iliuta and Larachi, 2002; Lakota et al., 2002; Nemec and Levec, 2005) and wetting efficiency (Augier et al., 2010; Baussaron et al., 2007a, 2007b;

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van Houwelingen et al., 2006). Previous experimental results have led to a better understanding of the real operating conditions of TBRs and the development of correlations that predict reactor hydrodynamic characteristics. Furthermore, mathematical models and numerical simulations of TBRs, which provide more details about process characteristics, have considerably improved. Numerical studies of TBRs, such as in experimental investigations, have been performed for a wide range of different operating conditions (Salimi et al., 2013; Bazmi et al., 2011a, b, 2012; Atta et al., 2007a, b, 2010; Gunjal et al., 2005, 2003; Gunjal and Ranade, 2007; Iliuta and Larachi, 2005; Iliuta et al., 2000a, b; Lappalainen et al., 2009; Lopes and Quinta-Ferreira, 2007, 2008, 2009, 2010a, b).

Evaluating the interfacial heat transfer in multiphase non-isothermal processes, such as TBRs, is one of the most significant areas of engineering science. Despite numerous studies on TBR hydrodynamics, few contributions have been made towards the understanding of TBR heat transfer fundamentals and the development of standardized correlations in this field (Habtu et al., 2011). Previously reported results include fundamental studied on the effective radial thermal conductivity (Borremans et al., 2003; Larachi et al., 2003; Mariani et al., 2003; Lamine et al., 1996), the wall-to-bed heat transfer coefficient (Habtu et al., 2011; Lamine et al., 1996; Larachi et al., 2003; Mariani et al., 2001) and the particle-to-fluid heat transfer coefficient (Borremans et al., 2004; Larachi et al., 2003; Marcandelli et al., 1999).

Although many experimental and numerical methods have been used to evaluate the heat transfer from wall-to-bed and particle-to-fluid, to the best of our knowledge, no study on the heat transfer at the gas–liquid interphase in TBRs has yet been completed. Interfacial heat transfer, especially between the gas and liquid phase, significantly effects phase properties and TBR reaction conversion. Therefore, the main goal of this study was to develop appropriate models that accurately describe the effects of various operating conditions and physical parameters on the interfacial heat transfer in TBRs. To complete this aim, two different models (micro-scale and meso-scale) were used to determine the geometry and hydrodynamic behavior of TBRs. The micro-scale model was developed based on the double-slit model (Iliuta et al., 2000a) and is a simplified description of the flow behavior in the trickle flow regime. The model was implemented to determine the interfacial heat transfer at different physical and operating conditions within the micro-scale domain. The micro-scale model accurately describes the hydrodynamic properties of TBRs. Additionally, low computational costs allow numerous studies to be completed on the effect of different operating conditions and physical phenomena on gas–liquid heat transfer. A second approach, the meso-scale model, was developed to account for the interfacial heat transfer of three different catalyst shapes (cylindrical, trilobe and spherical) using CFD techniques. This model is based on the VOF multiphase approach and was developed to examine the effects of operating parameters, such as particle shape, on the interfacial heat transfer. Moreover, an experimental study was performed to validate the CFD model at the meso-scale. The last section of this paper describes the development of a general correlation model that is based on our micro-scale model results and includes a study on a wide range of operating conditions and physical properties in the trickle bed reactor.

2. Experimental work

In this study, an experiment was designed to validate the CFD model, which is used to predict the distribution of gas temperatures during contact with the cold liquid film flowing around the wet catalysts. Fig. 1 is a schematic of the experimental setup. Fourteen spherical catalysts (with identical diameters of 40 mm) were loaded onto the bed axis (with a diameter 60 mm) in a vertical row. This arrangement of catalysts caused a symmetric flow. A 2D CFD domain was developed to reduce computational run time. Ambient air flowed over the top of the bed and cold water was uniformly distributed over the catalysts. It should be mentioned that all catalysts were subjected to a high flow rate of water prior to each experiment to achieve complete catalyst wetting. Additionally, the catalysts were covered with a thin plaster film to increase wettability. All experimental data were gathered at steady state conditions and each experiment was repeated five times to ensure repeatability of the results. Air flow velocity was measured by a SMART SENSOR AR856 anemometer with an accuracy of 0.001 m/s. The temperature profile in the gas phase was measured at five points along the bed using a Fluke 52 K/J digital thermometer with 0.1 °C accuracy.

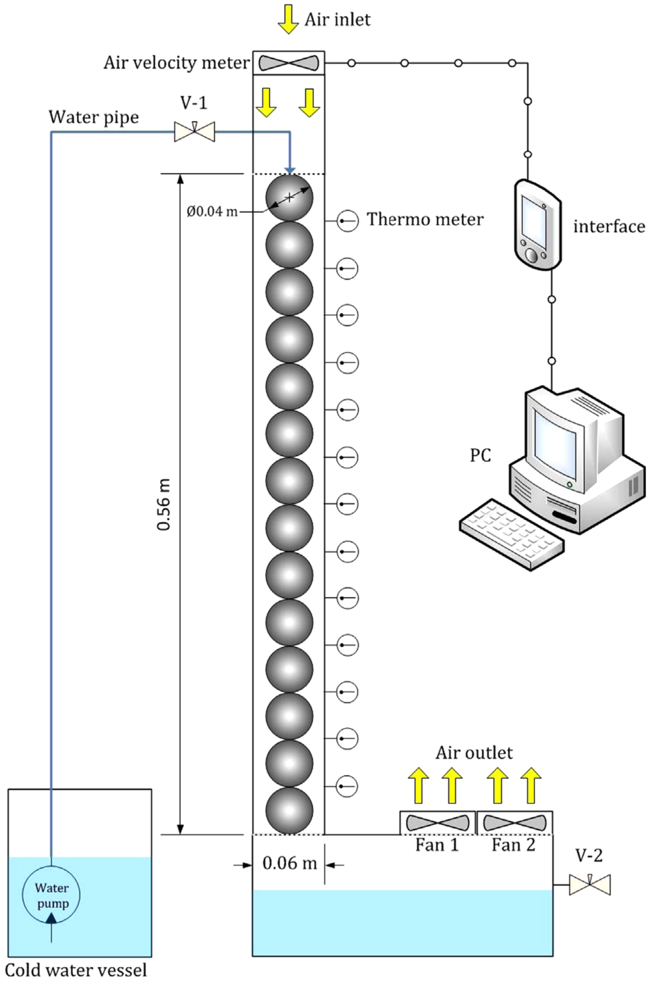

Fig. 1. Schematic diagram of experimental setup.

3. Model descriptions

The development of simple and reliable models is a major technique used to solve complex engineering and scientific problems. Because of complex geometries and multiphase flow conditions, the transport phenomena of TBRs are described by complicated mathematical models that must be simplified before solving. In the current study, two different methods were developed to evaluate the heat transfer at the gas–liquid interface of TBRs. The first method is based on the double-slit model (Iliuta