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Filtered model for the cold-model gas–solid flow in a large-scale MTO fluidized bed reactor

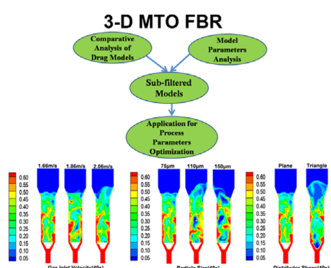
Li-Tao Zhu [a], Le Xie [a], Jie Xiao [b], Zheng-Hong Luo [a,*]

[a] Department of Chemical Engineering, College of Chemistry and Chemical Engineering, Shanghai Jiao Tong University, Shanghai 200240, PR China
[b] Suzhou Key Laboratory of Green Chemical Engineering, School of Chemical and Environmental Engineering, College of Chemistry, Chemical Engineering and Materials Science, Soochow University, Suzhou 215123, PR China

HIGHLIGHTS

- A filtered TFM is developed to model a commercial cold-model MTO FBR.
- Predictions are compared against data from classical models and experiments.
- Four CFD models under the same coarse-grid condition are compared.
- The dependence of filtered quantities on gas–solid flow in FBR is discussed.
- Filtered TFM is used to optimize MTO reactor operating conditions.

GRAPHICAL ABSTRACT



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ABSTRACT

In this work, a three-dimensional (3-D) filtered two-fluid model (TFM) was developed to describe the gas–solid flow behavior in a large-scale methanol-to-olefins (MTO) fluidized bed reactor (FBR). The cold-model flow behaviors were characterized successfully via the filtered TFM with a coarse grid. A coarse-grid sensitivity test was first carried out, and the filtered model was testified using predictions from classical models and the experimental data. Moreover, four drag models have been incorporated into the TFM for evaluating the effectiveness of these models at the same coarse-grid condition. Subsequently, the effects of some important model parameters including solid stresses, wall corrections and filter size on the flow behaviors were also investigated numerically. Finally, the filtered model was applied to predict the effects of the operating gas velocity, distributor shape and solid particle size. The results suggested the effectiveness of the sub-grid models for simulating large-scale MTO FBRs at coarse-grid conditions. This study further confirmed that the filtered drag coefficient correlation plays a significant role in capturing flow behaviors and the filter size is nearly independent on the grid size when the filter size is larger than or equal to twice the grid size. The simulation results by coarse-grid also show that the catalyst particles are easier to be fluidized with the increase of the operating gas velocity. It is also found that a triangle-shaped distributor strengthens the mixing behaviors and weakens the clustering of the near-wall regions. Additionally, our study indicates that the clustering phenomena near the wall regions are more obvious with the decrease of the catalyst particle size.

1. Introduction

CFD simulations of gas–solid flow in fluidized bed reactors (FBRs) with fine grids may suffer from the persistent fluctuations of flow field parameters and the high computational demands.

* Corresponding author. Tel./fax: +86 21 54745602.
E-mail address: luozh@sjtu.edu.cn (Z.-H. Luo).

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Thus coarse-grid simulation methods are usually desirable, which is especially true for large-scale FBR systems (Agrawal et al., 2001, 2013; Wang, 2009; Parmentier et al., 2012; Schneiderbauer et al., 2013). Unfortunately, such a procedure inevitably ignores small scales in gas and particle phases, which leads to inaccurate flow predictions (Agrawal et al., 2001; Andrews IV et al., 2005; Holloway and Sundaresan, 2014). In general, the effect of these small scales on the drag force is important for the accurate simulation of gas–solid flow (Holloway and Sundaresan, 2014). Therefore, filtered models have been suggested to consider the presence of small scale structure using sub-grid closures for fluid-particle drag force, particle phase stress, effective reaction rates, and heat transfer rates (Igci et al., 2008; Igci and Sundaresan, 2011a, 2011b; Holloway and Sundaresan, 2012, 2014; Agrawal et al., 2013; Schneiderbauer et al., 2013). Up to now, there has been considerable development of sub-grid models, including the energy-minimization multi-scale (EMMS) model and the filtered models. The EMMS group (Li and Kwauk, 1994; Yang et al., 2003; Wang and Li, 2007a; Wang et al., 2007b; Lu et al., 2009; Shi et al., 2011; Hong et al., 2012; Liu et al., 2015; Zhao et al., 2015), the Princeton's group (Igci et al., 2008, 2012; Igci and Sundaresan, 2011a, 2011b; Holloway and Sundaresan, 2012, 2014; Agrawal et al., 2013; Milioli et al., 2013; Radl and Sundaresan, 2014; Sarkar et al., 2013, 2014), the Simonin's group (Ozel et al., 2010, 2013; Parmentier et al., 2012), and the Austria's group (Schneiderbauer et al., 2012a, 2012b; Schneiderbauer and Pirker, 2014), are leading research groups in this field and have done excellent contributions to the development of sub-grid models. Schneiderbauer et al. (2013) reviewed previous contributions systematically in this field. In addition, up to now, all of these models have been applied to different flow systems including reacting gas-particle flows (Holloway and Sundaresan, 2012), bi-disperse cold-model gas-particle flows (Holloway and Sundaresan, 2014). However, to the best of our knowledge, the application of these filtered models to the methanol-to-olefins (MTO) process in large-scale FBRs has not been reported.

In practice, MTO reaction is one of the most significant reactions in C1 industrial chemistry. The MTO process in FBRs was realized successfully in China in 2010 (Zhang et al., 2010; Zhao et al., 2013; Tian et al., 2015), which provides a novel technology to produce key industrial products (like ethylene and propylene) from alternative and inexpensive nonoil-resources, such as coal and natural gas. Since then, the MTO process has been extensively investigated (Gayubo et al., 1996, 2000; Chen et al., 1999a, 1999b, 2000, 2007; Alwahabi and Froment, 2004a, 2004b; Aguayo et al., 2010; Park and Froment, 2001a, 2001b; Ying et al., 2015). However, most of these studies focused on the MTO catalyst and the MTO kinetics. Studies on the MTO process at the reactor scale are limited, particularly on the gas–solid flow behaviors in large-scale FBRs. Recently, Zhuang et al. (2012) developed a CFD model to describe the gas–solid flow behaviors in a MTO fixed-bed reactor. Chen et al. (2013) developed a direct concurrent multi-scale CFD model, which incorporates a single particle model and a two-phase CFD model, to predict the effects of intra-particle transfer on the flow field in a laboratory-scale FBR. A CFD model with fine-grid was constructed to characterize the gas–solid flow field in the FBR (Chen et al., 2013). Meanwhile, Zhao et al. (2013) applied a sub-grid CFD modeling approach to a 16 kt/a MTO FBR. In their model, the TFM was applied and the EMMS-bubbling model was selected to calculate the gas–solid drag force. In the same year, by incorporating a MTO kinetic model into the TFM, Chang et al. (2013) developed a reactor model for describing the gas–solid flow and reaction in a laboratory-scale FBR. More recently, Zhuang et al. (2014) suggested a combined discrete element method (DEM) and CFD model for describing the gas–solid flow behaviors in a laboratory-scale MTO FBR. The above studies addressed the importance of the CFD modeling technology in describing the gas–solid flow behaviors in FBRs. Additionally, based on the above discussions, it can be found that simulations of laboratory-scale MTO FBRs could be carried out using fine grid resolutions. Unfortunately, none of the above-mentioned efforts adopted the filtered TFMs with coarse-grid for large-scale MTO FBRs, which is obvious necessary for simulating large-scale reactors.

As a first step towards a comprehensive coarse-grid CFD modeling approach for a large-scale MTO reactor, herein, we applied a 3-D filtered TFM to describe the gas–solid flow behaviors at cold-model conditions. Firstly, the coarse-grid sensitivity and the validation of the filtered model were carried out. Four drag models, namely Wen and Yu, Gidaspow, EMMS and filtered drag, were also incorporated into the TFM for evaluating the effectiveness of these models under coarse-grid condition. Next, the effects of some important model parameters including solid stresses, wall corrections and filter size on the flow behaviors were also investigated numerically. Finally, the filtered model was used to explore the effects of the operating gas velocity, distributor shape and solid particle size on the flow behavior in the MTO FBR.

2. CFD model

2.1. TFM

The continuity equations for the gas-particle two-phase system can be written as:

$$\frac{\partial}{\partial t}(\alpha_g\rho_g)+\nabla\cdot(\alpha_g\rho_g\vec{v}_g)=0, \tag{1}$$

$$\frac{\partial}{\partial t}(\alpha_s\rho_s)+\nabla\cdot(\alpha_s\rho_s\vec{v}_s)=0 \tag{2}$$

where, subscripts g and s represent, respectively, the gas and solid phases. It is clear that

$$\alpha_g+\alpha_s=1. \tag{3}$$

The momentum conservation equations are

$$\frac{\partial}{\partial t}(\alpha_g\rho_g\vec{v}_g)+\nabla\cdot(\alpha_g\rho_g\vec{v}_g\vec{v}_g)=-\alpha_g\nabla p+\nabla\cdot\overline{\overline{\tau_g}}+K_{gs}(\vec{v}_s-\vec{v}_g)+\alpha_g\rho_g\vec{g}, \tag{4}$$

$$\overline{\overline{\tau}}_g=\alpha_g\mu_g(\nabla\vec{v}_g+\nabla\vec{v}_g^{\,T}), \tag{5}$$

$$\frac{\partial}{\partial t}(\alpha_s\rho_s\vec{v}_s)+\nabla\cdot(\alpha_s\rho_s\vec{v}_s\vec{v}_s)=-\alpha_s\nabla p-\nabla p_s+\nabla\cdot\overline{\overline{\tau_s}}+K_{sg}(\vec{v}_g-\vec{v}_s)+\alpha_s\rho_s\vec{g}, \tag{6}$$

$$\overline{\overline{\tau}}_s=\alpha_s\mu_s(\nabla\vec{v}_s+\nabla\vec{v}_s^{\,T})+\alpha_s\left(\lambda_s-\frac{2}{3}\mu_s\right)\nabla\cdot\vec{v}_s\overline{\overline{I}}. \tag{7}$$

In the filtered gas-particle model, variables above represent filtered values.

2.2. Closures

In this work, the kinetic theory of granular flow (KTGF) closure is employed when filtered closure is not required. Given that the KTGF has been documented in our group's previous publications (e.g. Gao et al., 2010; Chen et al., 2011; Yan et al., 2012), herein, it will not be presented in detail.

2.2.1. The classical models

The Gidaspow et al. (1994) model is implemented to describe the momentum transfer between the gas and solid phases, which