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Model-based analysis of the impact of the distributor on the hydrodynamic performance of industrial polydisperse gas phase fluidized bed polymerization reactors

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ABSTRACT

A two dimensionally Eulerian–Eulerian multiphase flow model coupled with a population balance modeling (CFD–PBM) simulation was implemented to investigate the fluidization structure in an industrial scale gas phase polymerization reactor (FBR). Direct quadrature method of moments (DQMOM) was employed in this model to solve the PBM. Two cases including perforated distributor and complete sparger have been applied to examine the flow structure through the bed. A simulation of the reactor with perforated distributor was performed first to validate and evaluate the impact of distributor's characteristics on the fluidization behaviors. The predicted results were in good agreement with the industrial data in terms of pressure drop and bed height. The results showed that different heterogeneous flow patterns were created in a perforated distributor, due to more kinetic energy and jet formation above the distributor. A dead zone is expected to be formed near the corners of the perforated distributor. In addition, the cluster formation is expected to be decreased in comparison with the complete sparger plate distributor. Furthermore, the results predicted bigger bubble diameter in the case of the perforated distributor by using an image processing technique. The information obtained from this study could be important to assure efficient industrial operations of FBRs.

1. Introduction

Considering the potentials of fluidized bed reactors (FBRs) to provide the favorable particle mixing, mass/heat transfer characteristics, and simple operation, they are widely exploited for numerous chemical industrial applications [1–3], especially for polymerization processes [4–8]. The former studies have shown that the efficiency of FBRs is related to reactor configuration, physical properties, superficial gas velocity, operation pressure/temperature, particle size distribution (PSD) and gas distributor [2,9]. Some techniques such as capacitance probes [10, 11], optical fiber [12], X-ray imaging [13], pressure transducers [14], particle image velocimetry [15], and magnetic resonance imaging [16, 17] have been used to obtain fluidization information. Recently, due to better accessibility to the high-performance computer technology and computational power, considerable attention has been paid to the implementation of computational fluid dynamics (CFD) for simulating the flow structure in the gas phase FBRs. However most of the reported simulations on the FBRs have been carried out with uniform inlet gas velocity (complete sparger in inlet boundary condition), many industrial FBRs exploit a distributor to uniformly distribute the gas-phase feed stream. In order to assure the optimum design, operation, the scale up of the FBRs, and a deep understanding of the impact of the distributor on the hydrodynamic aspects are necessary [18]. Therefore, from the industrial point of view, it is very important to predict the impact of the distributor on the performance of FBRs, accurately.

Although the distributor represents only a small part of the bed, a good distributor introduces uniform bubbles over the entire cross-section of the bed to reach effective rate of mass/heat transfer, flow pattern, prevention of particle fall back, particle attrition reduction and mixing. While, mal-distribution reduces the effective interfacial area and may result into particle agglomeration, distributor hole plugging, partial de-fluidization and weeping through part of distributor [15,19]. Many fundamental studies have been focused on the impact of distributor such as distributor hole pitch [15,20], opening area [21,22], perforated ratio of distributor [23], fluidization regime [24,25] and different types of distributor [19,26–28].

In order to predict the impact of distributor on the performance of FBRs, two different approaches, Eulerian–Lagrangian [6] and Eulerian–Eulerian [29–32], can be implemented. The Eulerian–Lagrangian model consists of a Newton's equation of motion of each particle by considering the particle–particle collisions and the resulted forces acting on the particle, and a continuous interpenetrating model for the gas phase. Due to the extensive requirements for computational efforts, the

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application of this method is limited only to the relatively pilot and laboratory fluidization systems. In the Eulerian–Eulerian model, the dispersed solid particles are also treated as an interpenetrating continuous fluid. Although, this method is faster than the Eulerian–Lagrangian method, while requires additional constitutive equations to describe the rheology of dispersed phase. Most authors [23,33–37] have been used Eulerian–Eulerian approach to simulate the dense gas–solid systems coupled with the kinetic theory of granular flow (KTGF). Recently considerable attention has been devoted to the implementation of the CFD modeling in gas-phase fluidized bed polymerization reactors. Most of the reported findings have analyzed a mono-dispersed solid phase [36,38], but some other researchers have performed the CFD analysis of bi-dispersed mixture to predict the mixing/segregation phenomena [39–42]. In reality, industrial FBRs are characterized by a broad range of PSD that change along the bed due to particle kinetics (growth, aggregation and breakage phenomena). Therefore it is very important to consider the impact of PSD on the performance of reactor [5,18,43–45]. One efficient method to analyze the impact of PSD on the performance of FBRs is by coupling the population balance model (PBM) into the CFD framework [5,18,46–48]. The main advantages of the CFD–PBM coupled model are:

a) It is able to predict the flow pattern (using CFD) and particle size distribution (using PBM).
b) It has the ability to consider the particle kinetics (growth, aggregation and breakage phenomena)
c) It is able to investigate the influence of the PSD on the flow structure in different regimes.

In order to analyze the flow structure in the multiphase gas phase FBRs, several hybrid CFD–PBM models have been proposed such as class method (CM) [49,50], method of moments (MOM) [51,52], standard method of moment (SMM) [53,54], quadrature method of moment (QMOM) [5,55], sectional quadrature method of moments (SQMOM) [56] and quadrature method of moments (DQMOM) [57,58]. Recently, the merits and demerits of these numerical techniques were summarized by Akbari et al. [46]. The method of moment (QMOM and DQMOM) has been specifically proposed to couple the PSD in CFD framework [52,57,59–61]. QMOM and DQMOM both approximate the density function with quadrature formulas and the main difference is related to obtaining the values of the quadrature nodes and weights [62,63]. DQMOM is based on the directly integrating transport equations for weights and abscissas of the quadrature approximation. QMOM, conversely, tracks the moments by integrating their transport equations and back-calculates node and weights. In addition, QMOM needs to run the product-difference (PD) algorithm in each time step and computational cell, while the DQMOM needs this additional computation only once, which is to initialize the quadrature nodes and weight [58]. Harshe et al. [64] developed a generic framework for the fluidized bed polypropylene reactor based on a mixing cell approach and polymerization kinetics coupled with PSD. Although this framework can be used to understand the impact of operating parameters on PSD, their procedure cannot take advantage of dynamic variations of PSD with respect to time. Yan et al. [5] coupled the population balance equation (PBE)/QMOM with a Eulerian–Eulerian model to simulate the fluidized bed polymerization reactor. Their results showed the acceptable agreement compared to the experimental data. Fan et al. [57] highlighted the potential of the DQMOM to solve the PBE which has been integrated into the CFD Eulerian–Eulerian framework to simulate the polydispersed gas–solid FBRs. In the DQMOM, considering of each node as an independent distinct solid phase has some advantages. However, Mazzei et al. [63,65] have pointed out that the QMOM and the DQMOM do not yield the same numerical results, and the QMOM is more accurate rather than the DQMOM. Ignoring the influence of the distributor on the fluidization structure is the most drawbacks of their studies.

The effect of the gas distributor on the fluidization behavior can be analyzed by using CFD simulation. Dong et al. [23] have investigated the particle concentration and bed pressure drop by changing the perforated ratios of distributor and they found that the bubble size decreases with increasing diameter of the perforated distributor. They have also observed that the pressure drop decreases with increasing the perforated ratio and superficial gas velocity. In addition, Jangam et al. [66] studied the impact of design specifications of the gas distributor to obtain a uniform distribution across the bed. They predicted that the flow pattern can be improved by reducing the percentage of the open area of distributor. Furthermore, they reported more uniformity of distribution with the increase of orifice diameter. The effect of hole size and superficial gas velocity on the bubble size distribution has been investigated using 2-D and 3-D models by Rampure et al. [67]. Their results showed a good agreement with the experimental data. In addition, Peng et al. [25] have applied a Eulerian–Eulerian multi–fluid model to analyze the effect of gas distributor and solid distributor in a circulating fluidized bed riser. They proposed two potential approaches to improve the uniformity of radial solid concentration profiles, by using a center-sparse side-dense air jet arrangement for the gas distributor, and also applying a side-covered arrangement concept for the solid distributor. In addition, Hosseini et al. [68] have modeled the 2-D Eulerian model to investigate the partial and complete sparger distributor. Their results illustrated that the CFD results could be improved by using a perforated distributor, while the modified partial sparger needs to properly improve the fluidization structure. A CFD model-based study of the effect of eight different gas distributors on the liquid velocity and gas hold-up, especially above the distributor, was provided by Li et al. [20]. According to their findings, a higher gas-hold up is predicted as a result of increasing the number of spargers, while the bubble diameters decrease due to lower turbulent kinetic dissipation. They also demonstrated that the mixing characteristic is improved with smaller gas sparger pipes. Recently, Şal et al. [19] have studied experimentally the effect of perforated distributor on gas holdup and regime transition points in bubble column. The total gas holdup was increased by decreasing the hole diameter in homogeneous flow regime while there is no significant effect in the heterogeneous regime. Therefore, it can be highlighted that the importance of analyzing the real behavior of distributor as well as PSD effects on the system's performance has been largely neglected in the previous hydrodynamic studies.

To our best knowledge, the application of an existing CFD–PBM/DQMOM coupled model to simulate the entrance configuration in industrial fluidized bed polymerization reactor has not been reported yet. The present work focuses on the application of CFD–PBM coupled model to comprehensively monitor the influence of existing perforated distributor on fluidization structure of industrial LLDPE gas phase polymerization reactor. The transient 2-D CFD–PBM model is solved with the DQMOM. In this context, the effect of distributor on the reactor performance aspects such as pressure drop, bed height, clustering, dead zone formation and radial void fraction is discussed in details. In addition, the effect of number of nodes, time step, drag coefficient and specularity coefficient is also investigated. The multi-fluid Eulerian–Eulerian model and the DQMOM model are briefly introduced as the first stage. The details of the simulation, such as geometry, initial and boundary conditions and relevant parameters are also provided. Then, the simulation results are validated by comparing with the available industrial data in terms of bed height and pressure drop. Finally, the fluidization structure was compared with a complete sparger inlet configuration as the most acceptable entrance boundary condition in CFD modeling.

2. Multiphasic CFD–PBM coupled model

A step by step CFD–PBM/DQMOM coupled modeling framework application of gas-phase polydispersed fluidized bed reactor was implemented to couple the PSD in a multi-fluid CFD framework. The CFD–PBM coupled model is a flexible platform and thus by changing the geometry and constitutive equation, its application can be extended to various polydisperse multiphasic FBRs. As shown in Fig. 1, the generic