CHEMICAL ENGINEERING RESEARCH AND DESIGN 88 (2010) 757–771

Contents lists available at ScienceDirect

Chemical Engineering Research and Design

journal homepage: www.elsevier.com/locate/cherd

DEM simulation of particle mixing in flat-bottom spout-fluid bed

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ABSTRACT

The particle mixing mechanism affects the rate of the process and the achievable homogeneity. This paper presents a numerical study of the particle motion and mixing in flat-bottom spout-fluid bed. In the numerical model, the particle motion is modeled by discrete element method (DEM) and the gas motion is modeled by κ–ε two-equation turbulent model. Validation with experiments is first carried out by comparing solid flow pattern and bed pressure drop at various gas velocities. Then, particle velocities, obtained from DEM simulations, are presented to reveal the mixing mechanisms. On the basic, the dependence of mixing index on the time and the effect of gas velocity on mixing and dead zone (stagnant solid) are discussed, respectively. The results indicate that the spouting gas is the driving force for the formation of particle circulation roll, resulting in the mixing. The convective mixing caused by the motion of circulation roll, shear mixing induced by the relative move of circulation rolls and diffusive mixing generated by random walk of particle among circulation rolls are three different mixing mechanisms in spout-fluid bed. The increase of spouting gas velocity promotes the convective and shear mixing. While increasing the fluidizing gas velocity improves significantly the convective mixing and but weakens the shear mixing. Both of them yield a reduction in the dead zone.

Keywords: Particle mixing; Circulation roll; Mixing mechanism; Spout-fluid bed; Mixing index

1. Introduction

A spout-fluid bed is a unique fluid-particle-agitated bed which combines a number of favorable properties of both spouted and fluidized beds. This technique has been accepted traditionally as a solid–fluid contacting method for physical operations such as drying, coating and granulation of granular solids (Link et al., 2004, 2007; Park et al., 2006; Plawsky and Littman, 2006; Zielinska and Markowski, 2007; Białobrzewskia et al., 2008). In recent years, the application of spout-fluid bed reactors has extended to catalytic reactors and combustion and gasification of coal and biomass (Lim et al., 1988; Arnold and Laughlin, 1992; Xiao et al., 2006; Zhong et al., 2006a,b).

Particle mixing is deemed as a complex process to obtain a uniform mixture of ingredients distributed among each other (Gyenis, 1999). In many industrial applications, the mixing and contacting of reactants and products very often are the controlling factors in the reactor performance since mixing is closely related to the rates of mass, heat and moment transfers. Good mixing among reactors is essential to avoid hot spots due to the heat released by the highly exothermic reactions and segregation of the larger particles at the bottom of reactor. Whereas poor homogeneity of the particulate mass can lower the overall process efficiency and complicate its thermal control.

Mixing mechanism, as a qualitative feature, characterizes the way of intermingling of components, which significantly influences the rate of the process and also the achievable homogeneity. So the detailed knowledge of the fundamental mechanisms is important to enhance the performance of operations. In addition, the mixing process acting during the practical operation depends on the operating condition to a great extent. Therefore, it is essential to identify the dominant mixing mechanism at different operating conditions, which helps to control the operation.

There is extensive literature (Rowe et al., 1965; Singh et al., 1972; Valenzuela and Glicksman, 1984; Fan et al., 1986; Lim et al., 1993; Shen and Zhang, 1998; Stein et al., 1998; Hoomans et

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Received 8 March 2009; Received in revised form 13 October 2009; Accepted 13 November 2009

doi:10.1016/j.cherd.2009.11.011

al., 2001; Rhodes et al., 2001; Bokkers et al., 2004; Lu and Hsiau, 2005; Wang et al., 2006; Feng and Yu, 2007; Tian et al., 2007) concerning the mixing in the conventional fluidized bed, most of which can be divided into two categories: specific numerical and experimental studies. The specific studies concern an experimental or numerical quantitative analysis of the mixing performance or dynamics. In the area of experiments, a couple of early methods (Rowe et al., 1965; Singh et al., 1972; Valenzuela and Glicksman, 1984; Fan et al., 1986; Yang et al., 1986; Lim et al., 1993; Shen and Zhang, 1998; Hoomans et al., 2001) have been employed to investigate the mixing, which provide some macroscopic information. Recently, some non-invasive measurement techniques (Stein et al., 1998; Bokkers et al., 2004; Wang et al., 2006) are developed to get some microscope information based on particle-scale. However, one of the problems of experimental investigation on particle mixing is that particle motion characteristic within the bed could not be obtained. Thus, systemic discussions engaged in the microscopic mixing phenomena of dense gas–solid flows, in temporal and spatial details, are believed unavailable. Generally computational models do not suffer from these limitations and some of them have reached a considerable maturity in correctly representing the phenomena involved in fluidization (Alberto et al., 2008). In recent years, numerical simulation has been widely used for studying gas–particle systems as it promises to be a useful tool for obtaining a wide range of flow properties of particles and gas flows simultaneously. Among these modeling approaches developed recently, discrete element method simulations (Rhodes et al., 2001; Lu and Hsiau, 2005; Feng and Yu, 2007; Tian et al., 2007) prove ideal to investigate the particle behaviour of fluidized beds.

In the DEMs there have been two types, i.e. the soft sphere models (Tsuji et al., 1993; Rikami et al., 1998; Rhodes et al., 2001) and the hard sphere models (Yuu et al., 1995; Hoomans et al., 1996). In the soft sphere models, particles are permitted to suffer minute deformation, and these deformations are used to calculate elastic, plastic and frictional forces between particles. In a hard sphere models, a sequence of collisions is processed and the forces between particles are not explicitly considered. Therefore, the force model is extremely important for DEM simulation. In gas–solid system, particle–fluid interaction forces must be properly considered except for the contact force and non-force induced by the collisions between particles or walls (Zhu and Yu, 2006; Zhu et al., 2009). These forces such as pressure gradient force, virtual mass force and Basset force tend to be ignored, particularly Saffman force and Magnus force.

Whether for experiment or numerical simulation, it is commonly considered that the axial and lateral motion of bubbles is the basic mechanism of particle mixing in fluidized bed. This may be summarized as follows. When a bubble rises through the bed, it carries a wake of particles to the bed surface and causes a drift of particle to be drawn up below it, which leads to the axial mixing. At the same time, the interaction and coalescence of neighboring bubbles causes the lateral motion of bubbles, resulting particle mixing in the lateral direction of the bed (Rhodes et al., 2001). While the mechanism of the solid mixing in the spouted bed is one of the fields on which many groups of investigators focused their interests. It is widely accepted that in the spouted bed most of the mixing action comes from the fountain and the spout (Kang and Mo, 1985; Larachi et al., 2003). For the spout-fluid bed operating at the low fluidizing gas velocity, however, there are no obvious bubbles occurring in the annulus. Accordingly, it is clear that mixing mechanism in spout-fluid bed is different from one in the ordinary fluidized bed. Up to now, however, the report at this respect has not been found in the literature.

In this paper, we perform DEM simulations to investigate the mixing mechanism in spout-fluid bed. It aims at better understanding particle mixing behavior in spout-fluid bed. The organization of current paper is as follows. As a first step, the DEM model and simulation condition will be described. Subsequently, experiment combining the bed-frozen method and image processing technology will be carried out in order to assess predicting ability of the model by comparing the simulated and measured results under comparable conditions in terms of solid flow pattern and bed pressure drop. Then, mean particle velocities, computed from DEM simulations, are presented and the mixing mechanisms in spout-fluid bed are determined combining the analysis of particle velocity and visual observation during the real experiments. Finally, the dependence of mixing index on the mixing time and the influences of gas velocity on the mixing and dead zone are fully discussed based on the elucidated mixing mechanisms.

2. Computational models and calculation conditions

2.1. Model

Details of the DEM model have been given by Zhong et al. (2006a,b) and only a very brief summary is presented here. In our previous study, this model has been used for investigation the gas–solid flow behaviors in spout-fluid bed.

2.1.1. Particle phase

In the present work, the particle motion is calculated three-dimensionally. In addition to the drag force, contact force and gravitational force, the shear induced Saffman lift force and rotation induced Magnus force are considered.

A particle in a granular flow can have two types of motion: translational and rotational. During its movement, the particle may interact with its neighboring particles or wall and interact with its surrounding fluid, which leads to the momentum and energy exchange. Newton's second law of motion can be used to describe the motion of individual particles, which can be written as:

$$m_p \frac{d\upsilon_p}{dt} = f_C + f_D + f_{LS} + f_{LM} + m_p g \tag{1}$$

$$I_p \frac{d\omega_p}{dt} = M_p \tag{2}$$

where υ_p and ω_p are the translational and angular velocities of particle, respectively, I_p and M_p are the particle moment of inertia and the particle torque, respectively, f_C and f_D are the contact forces among particles and drag force acting on particles, respectively, and f_{LS} and f_{LM} are the Saffman lift force and the Magnus lift force, respectively.

Contact forces are described in terms of a mechanical model involving a spring, dashpot and friction. Basically, the contact force has two components: normal and tangential, as follows:

$$f_C = f_{cnij} + f_{ctij} \tag{3}$$

$$f_{cnij} = (-k_n \delta_{nij} - \eta_n \upsilon_{tij} \cdot n_{ij}) n_{ij} \tag{4}$$