Chemical Engineering Science 65 (2010) 1462–1473

Contents lists available at ScienceDirect

Chemical Engineering Science

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

Numerical simulation of flow behavior of agglomerates in gas–cohesive particles fluidized beds using agglomerates-based approach

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ARTICLE INFO

Article history:
Received 18 January 2008
Received in revised form
3 October 2009
Accepted 21 October 2009
Available online 4 November 2009

Keywords:
Fluidization
Kinetic theory of granular flow
Agglomeration
Multi-phase flow
Cohesive particles
Numerical analysis
Simulation

ABSTRACT

Flow behavior of gas and agglomerates is numerically investigated in fluidized beds using a transient two-fluid model. It is assumed that the particles move as agglomerates rather than single particles in the gas–cohesive particles fluidized beds. The present model is coupled a modified kinetic theory model proposed by Arastoopour (2001) with an agglomerate-based approach (ABA). The interaction between gas and agglomerates is considered. The agglomerates properties are estimated from the ABA. Predictions are compared with experimental data measured by Jiradilok (2005) in a bubbling fluidized bed and Li and Tong (2004) in a circulating fluidized bed. The distributions of velocity, concentration and diameter of agglomerates, and pressure drop are numerically obtained. The influences of the contact bonding energy on the distributions of velocity and concentration of agglomerates are analyzed.

1. Introduction

Nanosized powders, such as ultrafine catalyst, ultrafine ceramic and ultrafine magnetic powders, have many attractive properties to industrial applications since these powders have advantages of high reaction rates and uniform microstructures, but easily agglomerated. Geldart (1973) divided particles into four groups (C, A, B and D) according to their fluidization characteristics. Ultrafine particles are in the Geldart-C group (cohesive powders). The fluidization behavior of cohesive particles was experimentally investigated (e.g., Chauoki et al., 1985; Morooka et al., 1988; Pacek and Nienow, 1990). Experiments observed that the cohesive particles in a fluidized bed exist in three states: unagglomerated single particles, natural agglomerates, and fluidized agglomerates. Li et al. (1999) indicated that the cohesive particles can be normally fluidized at agglomerates, and the size of agglomerates in a circulating fluidized bed (CFB) was smaller than that in a bubbling fluidized bed. The elutriation of cohesive particles from a fluidized bed was investigated (Li and Kato, 2001). The fluidizing behavior of Tullanox particles was experimentally studied by Jung and Gidaspow (2002) in a bubbling fluidized bed. An empirical correlation of stress modulus for Tullanox powders was proposed based on their experimental findings. Fluidization of SiO_2 nanoparticles showed a porous multi-stage agglomerate structure (Yao et al., 2002). Effect of sound on nanoparticle agglomerates, fluidization regime, minimum fluidization velocity, bed pressure drop, and bed expansion in a bubbling fluidized bed was investigated by Zhu et al. (2004). Experimental results indicated that with assistance of sound the nanoparticle agglomerates can be readily fluidized. The flow structures of channeling or slugging disappeared and the bed expanded uniformly. Effect of different particle interactions such as van der Waals, liquid bridging and electrostatic on different fluidization parameters was investigated by Hakim et al. (2005). Xu and Zhu (2005) investigated the agglomeration behavior of cohesive particles in fluidized beds with and without mechanical vibration. The experimental results indicated that the mechanical vibration can significantly reduce both the average size and the degree of the size-segregation of particle agglomerates throughout the bed.

Flow behavior of gas and particles can be numerically investigated using Eulerian–Eulerian two-fluid model or Eulerian–Lagrangian discrete particle trajectory model in fluidized beds. In Eulerian–Lagrangian particle trajectory model, gas is considered as the continuous medium and the particles are tracked in discrete Lagrangian coordinates from solving the particle motion equations with considering the effect of particle–particle interactions. Mikami et al. (1998) simulated the

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doi:10.1016/j.ces.2009.10.019

fluidized behavior of cohesive particles using a discrete numerical simulation model considering the effect of particle–particle interaction force. Helland et al. (1999) simulated the flow structure of cohesive powders in a riser based on an Eulerian–Lagrangian approach. Rhodes et al. (2001) analyzed the influence of the magnitude of the cohesive force of particles on fluidization characteristics in terms of the change in the ratio of the minimum bubbling to minimum fluidization velocities by a discrete element method. Kuwagi and Horio (2002) investigated the mechanism of agglomeration in a fluidized bed of cohesive particles by discrete element method. Effect of vibration on the cohesive particle motion in the fluidized bed was examined (Yuji et al., 2005; Limtrakul et al., 2007). On the other hands, Ding and Gidaspow (1995) and Jung and Gidaspow (2002) modeled, respectively, the fluidizing structures of cohesive particles in bubbling fluidized beds using the two-fluid model with results from kinetic theory of granular flow coupled with an empirical cohesive force model. Flow behavior of Geldart A particles was simulated on the basis of the two-fluid model (Ye et al., 2008). They found that a scale-down of the drag model is required instead of the Wen–Yu (1966) correlation in the simulations of fluidized beds. By defining a new distribution function of the instantaneous particle velocity relative to the average velocity based on the volume fraction of the particulate phase that was conserved upon agglomeration, Arastoopour (2001) and Kim and Arastoopour (2002) developed the governing equations of gas and cohesive particle flow using the kinetic theory of granular flow. The distributions of concentrations, velocity and agglomerate diameter of cohesive particles can be obtained by solving the derived conservation equations of mass, momentum, fluctuation energy, and particle number density.

In the present paper, flow behavior of gas and agglomerates is numerically simulated by a transient two-fluid model coupling with the gas–agglomerates interactions. It is assumed that the cohesive particles move as agglomerates rather than single particles in the fluidized beds. The modified constitutive relations of the particle phase are from kinetic theory for cohesive particles flow proposed by Arastoopour (2001). The agglomerates properties are predicted from an agglomerate-based approach (ABA). The distributions of velocity and concentration of agglomerates are numerically obtained. The effects of contact bonding energy of particles on flow behavior are analyzed. Simulation results are compared with experimental data of Jiradilok (2005) in a bubbling fluidized bed and Li and Tong (2004) in a circulating fluidized bed.

2. A two-fluid model of gas and agglomerates flow

Unlike Geldart B and D particles, two cohesive particles can be agglomerated by a collision. The agglomeration is directly related to surface properties of these two particles. The agglomerate is a group of cohesive particles joined together moving with the same velocity. In the agglomeration process, the kinetic energy dissipation is mainly attributed to surface cohesion of the particle–particle bindings, compared with the particle–particle inelastic collision. Arastoopour (2001) and Kim and Arastoopour (2002) developed conservation equations for fluidizations of cohesive particles by introducing the contact bonding energy E_c which is a function of the surface property of particles. The fluctuation energy or the granular temperature of particles is related to agglomerate–agglomerate collisions. The solids viscosity and pressure can be determined from computed granular temperature. In order to establish a mathematical model for flow of gas and particle agglomerates phases, we make the following assumptions: (1) the cohesive particle phase exists as spherical agglomerates. The gas flux through the agglomerates is neglected. As a first approximation, it is reasonable to ignore the gas velocity in the particle agglomerates. (2) The porosity in the agglomerates is assumed to be equal to zero, ε_a=0. This means that the sum of the concentration of gas phase ε_g and the concentration of agglomerates ε_s equals to unity $(\varepsilon_g+\varepsilon_a)+\varepsilon_s \approx \varepsilon_g+\varepsilon_s = 1.0$. (3) To account for the momentum transfer between the different size agglomerates due to collisions, the model requires constitutive relations known as agglomerate–agglomerate drag term. For simplifications, this drag term is neglected in present simulations. The authors recognize that in order to describe flow behavior of the different size agglomerates in gas–cohesive particles fluidized beds a multi-fluid Eulerian model is required. Based on above assumptions, the conservation equations of mass and momentum are re-formulated using the two-fluid approach. This approach treats gas and particle agglomerates as separate continuum phases. The governing equations for flow of gas and agglomerates phases, as well as the fluctuating energy of agglomerates are shown below.

2.1. Conservation of mass for gas and agglomerates phases

The mass balance equation of gas phase is expressed as follows:

$$\frac{\partial}{\partial t}(\rho_g \varepsilon_g)+\nabla\cdot(\rho_g \varepsilon_g \boldsymbol{u}_g)=0 \tag{1}$$

For agglomerates phase, the mass balance equation is

$$\frac{\partial}{\partial t}(\rho_s \varepsilon_s)+\nabla\cdot(\rho_s \varepsilon_s \boldsymbol{u}_s)=0 \tag{2}$$

2.2. Momentum equations of gas and agglomerates phases

The momentum balance for the gas phase is given by the Navier–Stokes equation, modified to include an interphase momentum transfer term

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g \boldsymbol{u}_g)+\nabla\cdot(\varepsilon_g \rho_g \boldsymbol{u}_g \boldsymbol{u}_g)= -\varepsilon_g \nabla p+\nabla\cdot\tau_g+\varepsilon_g \rho_g \boldsymbol{g} - \beta(\boldsymbol{u}_g-\boldsymbol{u}_s) \tag{3}$$

where τ_g is the viscous stress tensor of gas phase:

$$\tau_g=\varepsilon_g \mu_g[\nabla \boldsymbol{u}_g+\nabla \boldsymbol{u}_g^T]-\tfrac{2}{3}\varepsilon_g \mu_g \nabla\cdot u_g \tag{4}$$

The effective viscosity of gas phase μ_g is the sum of dynamic viscosity $\mu_{g,l}$ and turbulent viscosity $\mu_{g,t}$. The gas phase turbulence is modeled by the Sub Grid Scale (SGS) model, and thus the gas turbulent viscosity can be estimated as (Deardorff, 1971):

$$\mu_{g,t}=\rho_g(0.1\Delta)^2(\tau_g:\tau_g) \tag{5}$$

$$\Delta=(\Delta x\Delta y\Delta z)^{1/3} \tag{6}$$

For agglomerates phase, the momentum balance equation is

$$\frac{\partial}{\partial t}(\varepsilon_s \rho_s \boldsymbol{u}_s)+\nabla\cdot(\varepsilon_s \rho_s \boldsymbol{u}_s \boldsymbol{u}_s)= -\varepsilon_s \nabla p+\nabla\cdot\tau_s - \nabla p_s+\varepsilon_s \rho_s \boldsymbol{g}+\beta(\boldsymbol{u}_g-\boldsymbol{u}_s) \tag{7}$$

where τ_s is the viscous stress tensor of agglomerates phase,

$$\tau_s=\varepsilon_s\{\xi_s \nabla \boldsymbol{u}_s+\mu_s[(\nabla \boldsymbol{u}_s+\nabla \boldsymbol{u}_s^T)-\tfrac{2}{3}\nabla\cdot \boldsymbol{u}_s]\} \tag{8}$$

In present model, we use formulations for shear viscosity, μ_s, and bulk viscosity, ξ_s, given in Arastoopour (2001). For simplification, the complimentary error function is taken to be unity (Kim and Arastoopour, 2002). Because we focus on agglomerate contribution to flows, the particle diameter used in the original formulations of the kinetic theory of cohesive particles flow in Arastoopour (2001) is replaced by the agglomerate diameter.