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IMPROVED DEM-CFD MODEL AND VALIDATION: A CONICAL-BASE SPOUTED BED SIMULATION STUDY*

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Abstract: An improved and efficient DEM-CFD approach is developed for spouted beds. A nonlinear Discrete Element Method (DEM), with a concept of spring, dash-pot and friction slider, is used for tracing the movement of each individual particle. The gas flow is described by a set of reorganized governing equations. Two phases are coupled through contributions due to effects of porosity, viscosity and drag. All equations are solved with the commercial package Fluent with an implementation of User Defined Functions (UDF). To validate the improved model, a two-dimensional conical-base spouted bed is chosen as a case study. An unstructured mesh system is adopted instead of regular grid system. The simulation also takes the Saffman force and Magnus effect into account. The calculation results show good agreement with the experimental observations which are taken from the literature.

Key words: Discrete Element Method (DEM), spouted bed, Fluent User Defined Functions (UDF), unstructured mesh

1. Introduction

Spouted beds provide a means of good mixing of particles and gas-particle contacting for relatively large particles. The spouted bed technique has found applications in many industrial processes, such as catalytic cracking, tablets coating, combustion and granulations of fertilizers and other materials. The successful design and control of a spouted bed requires a better knowledge of the dynamics of the systems and the behaviors of each phase. An advanced experimental technique, such as the Particle Image Velocimetry (PIV), is an expensive approach to make a measurement of these properties. Theoretical studies of gas and solids motion in spouted bed have been conducted by many researchers. A characteristic common to most of these theoretical models is that all interaction forces between phases are lumped into one term through a special approach. The viscous stress terms for both phases are often neglected[1].

The approach based on a computer simulation has been widely used for studying dense particle systems, with an advantage of easily describing detailed and wide range flow properties[2-5]. In recent years, two most commonly used methods in the simulation of multiphase flows are the Two-Fluid Model (TFM) and the discrete element/particle method (DEM/DPM). The TFM approach treats the different phases as interpenetrating continua and a set of equations that have similar structure apply to each

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phase. For the DEM/DPM method, the gas phase is described by a locally averaged Navier-Stokes equation, while the motion of each individual particle is traced by a soft-sphere or a hard-sphere model, and two phases are coupled through a term due to inter-phase momentum transfer. Both approaches have been adopted in the simulations of spout beds. The hydrodynamic behavior in spouted bed was presented by many researchers[6-9] with a two-fluid gas-solids flow model. Huilin[10] and Wan[11] gintegrated a kinetic-frictional constitutive model for dense assemblies of solids in the simulation of spouted beds. The model treated the kinetic and frictional stresses of particles additively. Using the TFM method embedded in the commercial CFD simulation package Fluent, Du[12,13] described the influences of the drag coefficient correlations, frictional stress, maximum packing limit and coefficient of restitution of particles on the CFD simulation of spouted beds.

The TFM approach is more feasible for practical application to complex multiphase flows, however, it does not recognize the discrete character of the solid phase, and there has not yet been a quantitative analysis to assess multi-particle microstructures. The DEM/DPM approach offers a more natural way to simulate the systems of spouted bed with complex behavior. Several attempts have been made to model spouted beds using this approach[14-18]. One of the challenges confronting the solution of spouted bed is how to handle the convergence problem induced by the porosity variation. Additionally, one should also pay attention to the boundary condition at the conical surface for the V-shape spouted beds. Several researchers have developed the DEM simulations of a conical-base spouted bed under a regular grid system[19-22]. The accuracy of the simulations will not be guaranteed because additional closure equations are required for their boundary conditions.

In this article, an efficient DEM-CFD model is developed for the spouted beds. The model is incorporated into the commercial Fluent console with a method described by Wu[23,24]. The objective of the present work is to extend the previous simulation techniques under regular grid system to an unstructured mesh system. An advantage of our approach is that it can minimize codes modifications to adapt to spouted beds of arbitrary shape.

2. Governing equations

2.1 *Particle motion*

The motion of each individual particle in the system can be described by Newtonian second law of motion. Thus, at instant t, the translational and rotational motions of particle i with mass m_i and volume V_i are governed by

$$m_i \frac{\mathrm{d}\boldsymbol{u}_{pi}}{\mathrm{d}t} = -V_i \nabla p + \frac{V_i \beta}{1-\varepsilon}\left(\boldsymbol{u}_f - \boldsymbol{u}_{pi}\right) + \boldsymbol{f}_{ci} + m_i \boldsymbol{g} \tag{1}$$

$$I_i \frac{\mathrm{d}\boldsymbol{\omega}_{pi}}{\mathrm{d}t} = \boldsymbol{T}_i \tag{2}$$

where $\boldsymbol{f}_{ci}$ is the particle-particle contact force, β the inter-phase momentum transfer coefficient, $\boldsymbol{T}_i$ the summation of torque caused by the tangential components of the contact force, and I_i, and u_{pi} and $\boldsymbol{\omega}_{pi}$ are the moment of inertia, linear velocity and angular velocity, respectively, of the particle. The forces on the right side of Eq.(1) are respectively due to the pressure gradient, drag, inter-particle contact forces and gravity.

2.2 *Fluid motion*

The continuity and momentum equations for the fluid motion are based on local mean variables, given as

$$\frac{\partial\left(\varepsilon \rho_f\right)}{\partial t} + \nabla\bullet\left(\varepsilon \rho_f \boldsymbol{u}_f\right) = 0 \tag{3}$$

$$\frac{\partial\left(\varepsilon \rho_f \boldsymbol{u}_f\right)}{\partial t} + \nabla\bullet\left(\varepsilon \rho_f \boldsymbol{u}_f \boldsymbol{u}_f\right) = -\varepsilon \nabla p -$$

$$\nabla\bullet\left(\varepsilon \boldsymbol{\tau}_f\right) - \boldsymbol{S}_p + \varepsilon \rho_f \boldsymbol{g} \tag{4}$$

where $\boldsymbol{u}_f$, ρ_f and ε are the fluid velocity, density and the void fraction, respectively, $\boldsymbol{\tau}_f$ is the viscous stress tensor which is assumed to obey the general law for a Newtonian fluid:

$$\boldsymbol{\tau}_f = \left(\lambda_f - \frac{2}{3}\mu_f\right)\left(\nabla\bullet\boldsymbol{u}_f\right)\mathbf{I} + \mu_f \bullet$$

$$\left[\nabla\bullet\boldsymbol{u}_f + \left(\nabla\bullet\boldsymbol{u}_f\right)^{\mathrm{T}}\right] \tag{5}$$

where the bulk viscosity λ_f can be set to zero for gases.

The interaction between the gas phase and the particles is achieved via the coupling term $\boldsymbol{S}_p$, which is computed from