THREE-DIMENSIONAL GAS-SOLID FLUIDIZED BED SIMULATION APPLYING THE CFD TECHNIQUE

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Abstract

In this study, a three-dimensional two-phase flow model based on the kinetic theory of granular flow (KTGF) was used to predict the behavior of a gas-solid fluidized bed. The model is based on a Eulerian description of the two phases, gas and particles, and is composed of a set of mass conservation and momentum equations for each phase. In this model, the k-epsilon turbulence model and multiphase mixture are used. In order to describe the behavior of several particles in a continuum, the kinetic theory of granular flow was used.

The geometry and numerical mesh were generated using ANSYS ICEM CFD software and the set of partial differential equations was discretized and solved using CFX. Simulation data were verified against data found in Samuelsberg and Hjertager (1996), who used a cold flow laboratory circulating fluidized bed and simulated a two-dimensional model. Results using this model show that the model agrees with the experimental data and predicts a flow behavior similar to that found experimentally. It predicts the core annulus flow, which is known from the literature.
Keywords: Fluidized bed, CFD, Multiphase flow, Kinetic theory

Introduction

Fluidized beds are widely used in many operations in chemical, metallurgical, energy generation and especially petrochemical industries. Major applications are fluid catalytic cracking (FCC) risers and CFB combustor systems. Although fuidized beds are successfully and widely used in commercial industrial operations, much remains to be done due to the complexity of the gas-solid flow. No analytical tools that describe the influences of complex geometries, chemical reaction, internal reflux and heat transfer on the flow pattern in fluidized beds are available. With the increased availability of computers, mathematical models have been applied to predict the behavior of a fluidized bed and several models have been proposed. Gidaspow *et al.* (2004) carried out an extensive review of the models developed for the fluidized bed reactors and Peirano and Leckner (1998) reviewed turbulent gas-solid flow modeling in circulating fluidized beds.

Gas-particle two-fluid models, which treated the particle phase as a continuous fluid based on the Eulerian method, were widely employed in modeling gas-solid flow in the past several decades. A fundamental problem encountered in modeling the hydrodynamics of a gas-solid fluidized bed by the two-fluid method is how to include the stress of the particle phase in the particulate momentum equation. In the more recent two-fluid models, for the particle phase in dense gas-particle flow, the kinetic theory of granular flow has received attention and its use in Eulerian simulations has increased

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(Jenkins and Savage, 1983; Ding and Gidaspow, 1990; Gidaspow, 1994; Hrenya and Sinclair, 1997; Samuelsberg and Hjertager, 1996). The kinetic theory of granular flow is based on the kinetic theory of gases, first developed by Chapman and Cowling (1970). In this theory, the inter particle interactions are taken into account by adding the contribution of collisions between particles (Jenkins and Savage, 1983), which are the main mechanism of transport due to particulate phase properties.

The present study aims to simulate a three-dimensional two-phase flow model, based on the kinetic theory of granular flow (KTGF), to predict the behavior of a gas-solid fluidized bed, using a computational fluid dynamics technique.

Mathematical Model

Based on Eulerian description of the phases, a multiphase computational fluid dynamics model for turbulent gas-solid flow is presented. The Eulerian approach considers the two phases, gas and solid, as a continuum. The conservation equations for the solid phase are based on the kinetic theory for granular flow (Gidaspow, 1994).

The governing equations for transient three-dimensional gas-solid flow are presented as follows:

The continuity equation for phase i (= g,s):

$$\frac{\partial}{\partial t}\left(\varepsilon_i \rho_i\right) + \nabla \cdot \left(\varepsilon_i \rho_i \vec{\upsilon}_i\right) = S_i^{\rho} \tag{1}$$

where the subscript i can denote gas or solid phase, ε is the volume fraction, ρ is the density, t is the time, $\vec{\upsilon}$ is the velocity vector and S^{ρ} is the source term for mass transfer between the phases. Hence, no mass transfer is allowed between the phases.

The gas phase momentum equation:

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g \vec{\upsilon}_g\right) + \nabla \cdot \left(\varepsilon_g \rho_g \vec{\upsilon}_g \vec{\upsilon}_g\right) = -\varepsilon_g \nabla p_g + \nabla \vec{\tau}_g + \varepsilon_g \rho_g \vec{g} + \beta_{gs}^{m}\left(\vec{\upsilon}_s - \vec{\upsilon}_g\right) \tag{2}$$

where $\vec{g}$ is the gravity vector, p is the pressure and β_{gs}^{m} is the two-phase drag coefficient.

The stress tensor of the gas phase can be written as

$$\vec{\tau}_g = \varepsilon_g \mu_g \left(\left(\nabla \vec{\upsilon}_g + \left(\nabla \vec{\upsilon}_g\right)^T\right) - \frac{2}{3}\left(\nabla \cdot \vec{\upsilon}_g\right)\vec{I} \right) \tag{3}$$

Here, μ is the shear viscosity.

The gas phase turbulence is modeled with the k-epsilon model.

The solid phase momentum equation:

$$\frac{\partial}{\partial t}\left(\varepsilon_s \rho_s \vec{\upsilon}_s\right) + \nabla \cdot \left(\varepsilon_s \rho_s \vec{\upsilon}_s \vec{\upsilon}_s\right) = \nabla \vec{T}_s + \varepsilon_s \rho_s \vec{g} + \beta_{gs}^{m}\left(\vec{\upsilon}_g - \vec{\upsilon}_s\right) \tag{4}$$

where the solid stress tensor, $\vec{T}_s$, is the sum of a collisional part and a kinetic part and may be formulated as

$$\vec{\tau}_s = \left(-p_s + \lambda_s \nabla \cdot \vec{v}_s\right)\vec{I} + \mu_s\left(\left(\nabla \vec{v}_s + \left(\nabla \vec{v}_s\right)^T\right) - \frac{2}{3}\left(\nabla \cdot \vec{v}_s\right)\vec{I}\right) \tag{5}$$

where λ_s is the solid phase bulk viscosity.

The total solid phase pressure, p_s, consists of two terms; one of them, p_s^{k+t}, is determined from Lun *et al.* (1984) and includes both kinetic and collisional pressures, as follows:

$$p_s^{k+t} = \rho_s \varepsilon_s \left[1 + 2(1+e)\varepsilon_s g_o\right]\theta \tag{6}$$

where e is the coefficient of restitution and g_o is the radial distribution function.

The other term, p_s^f, is caused by friction and collisions in the solid phase due to highly dense flow, as proposed by Johnson and Jackson (1987), as follows:

$$P_s^f = Fr\frac{\left(\varepsilon_s - \varepsilon_{s,min}\right)^n}{\left(\varepsilon_{s,max} - \varepsilon_s\right)^p} \tag{7}$$

where the values of the constants in Equation (7) are Fr = 0.05, n = 2, p = 3 and $\varepsilon_{s,min}$ = 0.55, as suggested by Van Wachen (1998).

The total solid phase pressure is then given by

$$P_p = P_p^{k+t} + P_p^f \tag{8}$$

The radial distribution function, adopted by Lun and Savage (1986), is

$$g_o = \left(1 - \frac{\varepsilon_s}{\varepsilon_{s,max}}\right)^{-2.5\varepsilon_{s,max}} \tag{9}$$

where $\varepsilon_{s,max}$, the maximum particle packing chosen is 0.62.

Equation (9) is appropriate for dilute flow.

In Equation (6), θ is the granular temperature related to the kinetic turbulent energy of the particle motion. Ding and Gidaspow (1990) proposed the following equation for granular temperature:

$$\theta = \frac{1}{15(1-e)}d_p^2\left(\frac{1}{2}\left(\nabla \vec{v}_s + \left(\nabla \vec{v}_s\right)^T\right)\right) \tag{10}$$

where d_p is the particle diameter.

Solid phase bulk viscosity, λ_s, due to particle collisions (Lun *et al.*, 1984) and solid phase shear viscosity, μ_s, for dense and dilute flow (Hrenya and Sinclair, 1997) are given by the following equations:

$$\lambda_s = \frac{4}{3}\varepsilon_s^2 \rho_s d_s g_o (1+e)\sqrt{\frac{\theta}{\pi}} \tag{11}$$

$$\mu_s = \frac{5\sqrt{\pi\theta}}{96}\rho_s d_s\left[\left(\frac{1}{1+\frac{\lambda_{mfs}}{R}}\frac{1}{\eta g_o} + \frac{8\varepsilon_s}{5}\right)\left(\frac{1+\frac{8}{5}\eta(3\eta-2)\varepsilon_s g_o}{2-\eta}\right) + \frac{768}{25\pi}\eta\varepsilon_s^2 g_o\right] \tag{12}$$

where λ_{mfs} and η are given by

$$\lambda_{mfs} = \frac{d_p}{6\sqrt{2}\varepsilon_s} \tag{13}$$

$$\eta = \frac{1}{2(1+e)} \tag{14}$$

The gas-solid drag coefficient when $\varepsilon_g \leq 0.8$ is based on the Ergun equation and is given by

$$\beta_{gs}^{m} = 150\frac{\varepsilon_s^2 \mu_g}{\varepsilon_g d_p^2} + 1.75\frac{\left|\vec{v}_s - \vec{v}_g\right|\varepsilon_s \rho_g}{d_p} \tag{15}$$

And when $\varepsilon_g > 0.8$, based on the Wen and Yu equation:

$$\beta_{gs}^{m} = \frac{3}{4}C_D\frac{\left|\vec{v}_s - \vec{v}_g\right|\varepsilon_s \rho_g}{d_p} f(\varepsilon_g) \tag{16}$$

where $f(\varepsilon_g) = \varepsilon_g^{-2.65}$, as used by Gidaspow and Ettehadieh (1983).

The drag coefficient, C_D, is related to the Reynolds number as follows:

$$C_D = \varepsilon_g^{-2.65}\max\left[\frac{24}{Re_p\,\varepsilon_g}\left(1+0.15(Re_p\,\varepsilon_g)^{0.687}\right)\right] \text{ for } Re_p < 1000 \tag{17}$$

$$C_D = 0.44 \text{ for } Re_p \geq 1000 \tag{18}$$

$$Re_p = \frac{\left|\vec{v}_s - \vec{v}_g\right|\rho_g d_p}{\mu_g} \tag{19}$$

Results and Discussion

In order to validate the present numerical results, we compared them with the experimental results of Samuelsberg and Hjertager (1996). Then the simulations were carried out for the riser section of a circulating fluidized bed similar to that used by Samuelsberg and Hjertager (1996) and Mathiesen *et al.* (2000), shown in Figure 1 (a). In this study, just the riser section was simulated. The riser section is 1m high with an inner diameter of d = 0.032m. A secondary air supplier, positioned 0.05m above the gas inlet, feeds the solid back into the riser. The secondary gas inlet and the gas outlet have a diameter of 0.008m (Figure 1 (b)).The initial bed height is 0.05m and the initial solid volume fraction is 0.61. The system properties are defined in **Table 1**.

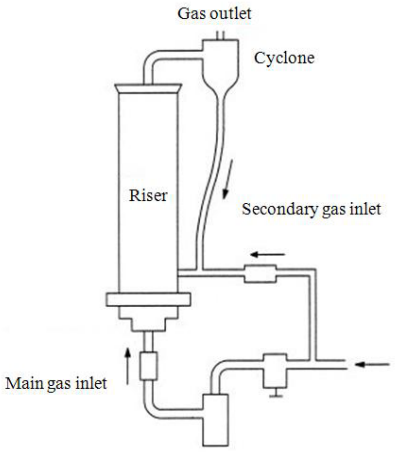
The riser section, as shown in Figure 1 (b), is modeled and simulated in a three-dimensional Cartesian coordinate system. Numerical predictions were obtained using the finite volume approach through the CFX-10 code, a CFD software developed by ANSYS, and the ICEM CFD code to generate the numerical grid, shown in Figure 1 (b). Numerical tests were conducted in order to optimize the computational grid. A grid of 300,000 control volumes was considered satisfactory considering the

precision of the results (10^{-4}) and the computation time consumed. The time step used in all simulations was 10^{-3}s.

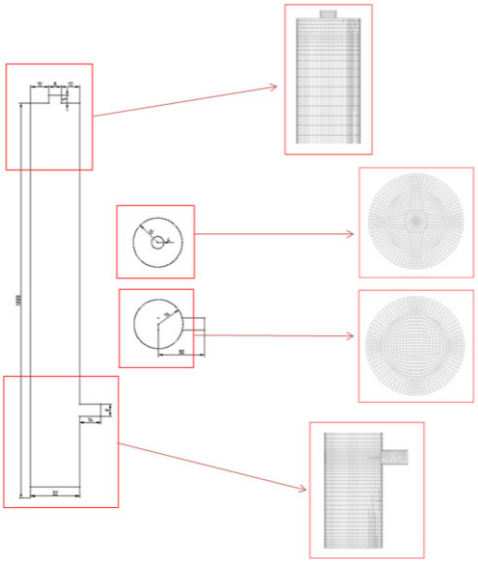
At the primary gas inlet, the superficial gas velocity, V_{sup}, was 0.71m/s. At the secondary gas inlet, the gas velocity and volume fraction were 0.05m/s and 0.6, respectively, and the particle volume fraction was 0.4. In order to permit all particles at the outlet back into the riser at the secondary gas inlet, a subroutine was implemented in the CFX code. At the outlet, atmospheric pressure was prescribed. At the walls, no-slip conditions were used for the solid phase as well as the gas phase.

The simulation results were computed through time-averaged distribution of flow variables. All the simulations were run for 7s of real time. To compute the granular temperature, solid-phase pressure and solid-phase bulk and shear viscosity must be programmed into the CFD codes due to the fact that the models used in this study were not presents in the CFX-10.

Figure 2 show a comparison of experimental results due to Samuelsberg and Herjtager (1996) and the present numerical results to the solid radial velocity profiles for heights of 0.16, 0.32 and 0.48m in the riser section and superficial gas velocity, V_{sup}, of 0.71m/s and 1.42m/s in the primary gas inlet.



(a)



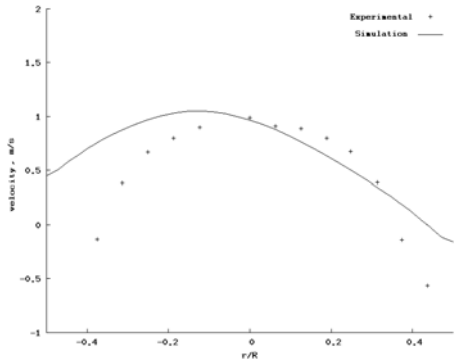
(b)

Figure 1 – (a) Geometry of Mathiesen *et al.* (2000). (b) Calculation domain and grid nodes

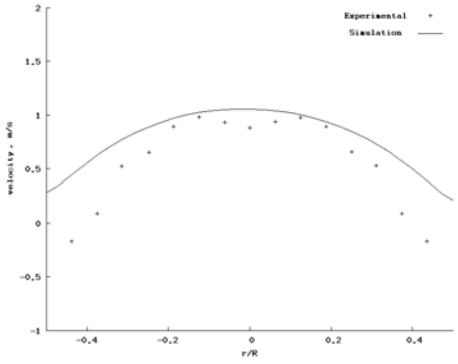
Table 1 – System properties

Gas density	1.185kg/m^3
Particle density	1600kg/m^3
Particle size	60μm
Gas viscosity	1.831x10^{-5}kg/m s
Maximum solids volume fraction	0.62
Particle-particle restitution coefficient	0.95

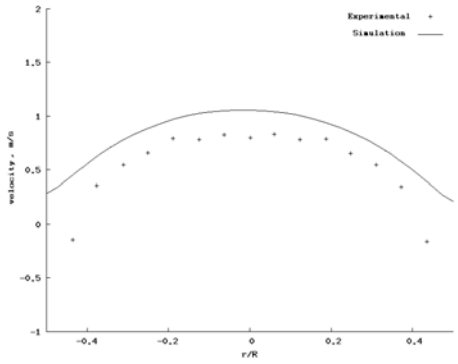
As can been seen in Figure 2 (b), (c), (e) and (f), the agreement is very good in the central region for all heights. The particles move upward in the central part of the riser and downward near the walls, a behavior well known from the literature, which is typical of core-annulus flow. However, in Figure 2 (a) and (d), for the height of 0.16m, the agreement between the curves differs significantly. These differences can probably be attributed to the region, both for the height of 0.16m, being so close to the secondary inlet, causing large perturbations in the flow. In Figure 2, a significant difference can be observed in the wall region for all results compared. This result may indicate that the no-slip wall boundary condition for both phases is not correctly used when employing KTGF.



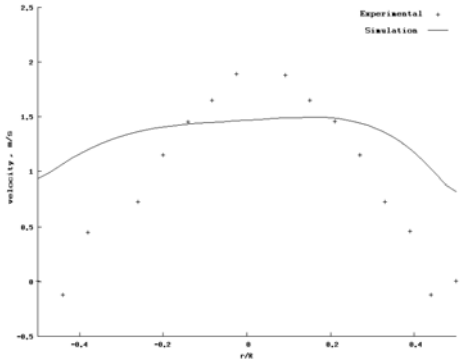
(a) Height of 0.16m and V_{sup} = 0.71m/s



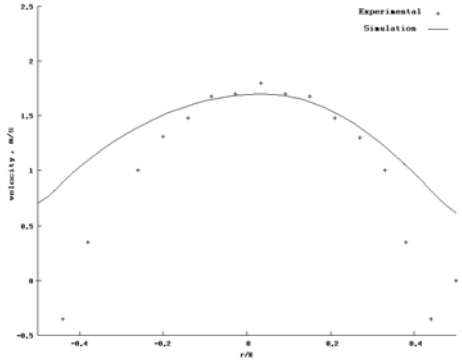
(b) Height of 0.32m and V_{sup} = 0.71m/s



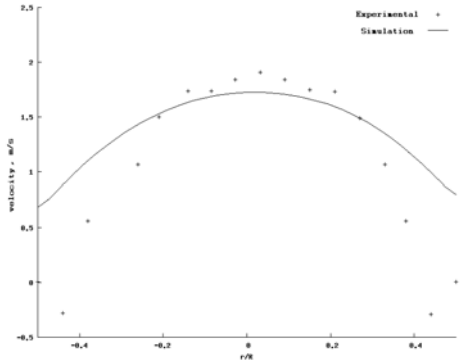
(c) Height of 0.48m and V_{sup} = 0.71m/s



(d) Height of 0.16m and V_{sup} = 1.42m/s



(e) Height of 0.32m and V_{sup} = 1.42m/s



(f) Height of 0.48m and V_{sup} = 1.42m/s

Figure 2 – A comparison of experimental data due to Samuelsberg and Herjtager (1996) and computed solid velocity profiles at different heights in the riser section and superficial gas velocity, V_{sup}, of 0.71m/s and 1.42m/s.

Conclusions

A three-dimensional two-phase flow model based on the kinetic theory of granular flow (KTGF) was used to predict the behavior of a gas-solid fluidized bed. The numerical results are compared against the experimental results of Samuelsberg and Hjertager (1996). The agreement is found to be satisfactory in the riser central region. However, in the wall region, the numerical results indicated a significant difference between all results compared.

References

1. Chapman, S., Cowling, T.G. (1970). *The Mathematical Theory of Non-Uniform Gases*, Cambridge University Press, London.
2. Ding, J., Gidaspow, D. (1990). A bubbling fluidization model using kinetic theory of granular flow. *AICHE J.*, 36, 523-538.
3. Gidaspow, D. (1994). *Multiphase Flow and Fluidization*, Academic Press, London.
4. Gidaspow, D., Ettehadieh, B. (1983). Fluidization in two-dimensional beds with a jet. 2. hydrodynamic modeling. *Industrial and Engineering Chemistry Fundamentals*, 22, 193-201.
5. Gidaspow, D., Jung, J., Singh, R.K. (2004). Hydrodynamics of fluidization using kinetic theory: an emergin paradigm 2002 flour-daniel lecture. *Powder Technology*, 148, 123-141.
6. Hrenya, C.M., Sinclair, J.L. (1997). Effects of particle-phase turbulence in gas-solids flows. *AIChE Journal*, 43, 853-869.
7. Jenkins, J.T., Savage, S.B. (1983). A Theory for the rapid flow of identical, smooth, nearly elastic, spherical particles. *AIChE Journal*, 42, 1536-1546.
8. Johnson, P.C., Jackson, R. (1987). Frictional-collisional constitutive relations for granular materials, with application to plane shearing. *Journal of Fluid Mechanics*, 176, 67-93.
9. Lun, C.K.K., Savage, S.B. (1986). The effects of an impact velocity dependent coefficient of restitution on stresses developed by sheared granular materials. *Acta Mechanica*, 63, 15-44.
10. Lun, C.K.K., Savage, S.B., Jeffrey, D.J., Chepurniy, N. (1984). Kinetic theories for granular flow: inelastic particles in couette flow and slightly inelastic particles in a general flowfield. *Journal of Fluid Mechanics*, 140, 223-256.
11. Mathiesen, V., Solberg, T., Hjertager, B.H. (2000). An experimental and computational study of multiphase flow behavior in a circulating fluidized bed. *International Journal of Multiphase Flow*, 26, 387-419.
12. Peirano, E., Leckner, B. (1998). Fundamentals of turbulent gas-solid flows applied to circulating fluidized bed combustion. *Progress Energy Combustion Science*, 24, 259-296.
13. Samuelsberg, A., Hjertager, B.H. (1996) Computational modeling of gas/particle flow in a riser. *AIChE Journal*, 42, 1536-1546.
14. VanWachen, B.G.M. (1998). Derivation, Implementation and Validation of Computer Simulation Models for Gas-Solid Fluidized Beds, PhD Thesis - Delft University.15.
15. Wen, C.-Y., Yu, Y.H. (1966). Mechanics of Fluidization. *Chem. Eng. Prog. Symp. Series*, 62,100-111.