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Simulation of rectangular fluidised bed with Geldart D particles.

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SIMULATION OF RECTANGULAR FLUIDIZED BED WITH GELDART D PARTICLES

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ABSTRACT

In this study, simulations are carried out using the Euler-Euler granular model in STAR-CCM+ for a gas-solid flow in a rectangular bubbling fluidized bed. The problem studied was announced as Small Scale Challenge Problem (SSCP-I) in 2013. Experiments for this problem were conducted by The Department of Energy's (DOE) National Energy Technology Laboratory (NETL). The objective of this numerical study is to evaluate the reliability of the kinetic theory based granular model (KTGF) in predicting the hydrodynamics of gas-solid flows.

The experimental measurements of the bubbling fluidized bed investigated in this numerical study are 3"x9"x48". The bed material for the experiment is Geldart group D particles of uniform size and high sphericity. Simulations were performed for all the three gas superficial velocities (U = 2.19, 3.28 and 4.38 m/s) for which experiments were conducted. Results from numerical simulations are validated for vertical component of particle velocity, horizontal component of particle velocity, granular temperature and the mean axial pressure gradient. The effect of the treatment at wall boundaries and coefficient of restitution (particle-particle interactions) is studied on the results.

Keywords: Fluidization, Bubbling fluidized bed, Geldart D particle, Kinetic theory of granular flow

NOMENCLATURE

Greek Symbols

α	Volume fraction.
ρ	Density, [kg/m^3].
τ	Stress Tensor, [kg/ (m.s^2)].
μ	Viscosity, [kg/(m.s)].
θ	Granular temperature [m^2/s^2].
γ_s	Collisional dissipation rate, [kg/ (m.s^2)].
φ	Specularity coefficient.

Latin Symbols

$\boldsymbol{U}$	Superficial velocity, [m/s].
p	Pressure, [Pa].
$\boldsymbol{u}$	Velocity, [m/s].
$\boldsymbol{g}$	Gravity, [m/s^2].
F	Force, [N].
d	Particle diameter, [m].
Re	Reynolds Number.
$\boldsymbol{c}$	Fluctuating velocity, [m/s].
e	Coefficient of restitution.
k	Granular conductivity, [kg/(m.s)].
J	Work done by fluctuating force, [kg/ (m.s^2)].
g_o	Radial Distribution Function.
A	Interphase momentum coefficient [kg/ (m^3.s)].
n	normal [m].
z	height measured from the inlet [m].

Sub/superscripts

mf	minimum fluidization.
i	i-th phase.
g	gas phase.
s	solid phase.
int	interaction.
b	bulk.
k	kinetic.
max	maximum packing limit.
$slip$	slip.
w	wall.

INTRODUCTION

Fluidized beds are widely used in many plant operations in chemical, energy production, oil & gas, mineral and agricultural industries. They are used widely because of their good mixing characteristics and high contact surface area between gas and solid phases.

The complex flow patterns associated with them make flow modelling of these systems a challenging task. The fundamental problem arises due to complex motion of phases where interface is unknown and transient, and interaction is understood only for limited range of conditions (Gilbertson *et al.*, 1996). Gas velocity and coefficient of restitution have significant impact on the hydrodynamic behaviour of the fluidized beds. CFD has emerged as an effective tool for modelling hydrodynamics of a fluidized bed. Mainly two approaches have been used to model gas – solid fluidized beds: Lagrangian approach, which tracks discrete particles and Euler-Euler approach where both phases are treated as interpenetrating continua. Gera *et al.* (1988) compared both these approaches.

In the Lagrangian approach, equations of motions are solved for each discrete particle and collisions between particles are modelled via hard-sphere (Gera *et al.*, 1988, Hoomans *et al.*, 1996) or soft-sphere approach (Tsuji *et al.*, 1993, Kobayashi *et al.*, 2000). But this approach is computationally very expensive and hence its usage is limited to problems with smaller number of particles. This makes Euler-Euler approach being more widely used to simulate gas – solid fluidized beds.

In Euler-Euler approach, particles are treated as a continuous medium. Governing equations are solved for each phase to ensure conservation of their continuity, momentum and energy. The interactions between the gas and solid phases appear as additional source terms in the conservation equations. The interphase momentum transfer between gas and solid phase is accounted for by the drag force. In fluidized beds, drag is affected by the presence of other particles. Many researchers, Wen *et al.* (1966), Syamlal *et al.* (1987), Arastoopour *et al.* (1990) and Di Felice, (1994) have proposed correlations for modelling drag for gas – solid flows.

The particle phase momentum equations require closure laws for additional terms that represent the rheology of the fluidized particles. Kinetic theory of granular flow was developed by Lun *et al.* (1984), Ahmadi *et al.* (1986) and Ding *et al.* (1990) to model the motion of a dense collection of spherical particles. This theory is based on the assumption that the motion of particles is analogous to random motion of molecules in a gas. Kinetic theory introduces a concept of granular temperature which represents the specific energy associated with fluctuations in velocity of particle about the mean. In gas-solid flows, fluctuations in the velocity result in collisions between particles which are being carried along by the mean flow.

In this study we focus on the Eulerian approach and investigate the impact of coefficient of restitution on the hydrodynamics of fluidized bed. Coefficient of restitution quantifies the elasticity of particle collisions. It takes value of one for fully elastic collisions and zero for fully inelastic collisions. Jenkins *et al.* (1983) were the first to account for loss of energy due to collision of particles. A number of studies have shown the effect of coefficient of restitution on the hydrodynamics of gas - solid flows (Goldschmidt *et al.*, 2001, Taghipour *et al.*, 2005 and Zimmermann *et al.*, 2005).

The objective of this study is to investigate the effect of coefficient of restitution and wall boundary treatment of particle phase on the hydrodynamics of a bubbling fluidized bed.

EXPERIMENT DETAILS

The bubbling fluidized bed system investigated in this study was declared as a challenge problem, Small Scale Problem – I (SSCP-I) by NETL in 2013 (Gopalan *et al.*, 2013). This system is a rectangular (pseudo 2-D) fluidized bed (3"x9"x48") using Geldart D type particles (Nylon beads). Experiments were performed at three different gas superficial velocities, $\mathbf{U}_g$ = 2.19, 3.28 and 4.38 m/s. The minimum fluidization velocity of the system, $\mathbf{U}_{mf}$ is 1.05 m/s. The mean particle size is 3.256 mm.

The data was collected for pressure drop across the bed, vertical and horizontal particle phase velocities and the granular temperature at 5 locations across the radius at 0.076 m distance downstream of the inlet. Additional details of the experiments can be found at Gopalan *et al.* (2013).

MODEL DESCRIPTION

In Euler-Euler model, each phase has its own distinct velocity, temperature and physical properties. Conservation equations are solved for each phases, but additional closure laws are required to model the interactions between the phases.

STAR-CCM+ solves the continuity and momentum equation for each phase, i. The conservation equations for mass and momentum take the following form,

Continuity:

$$\frac{\partial}{\partial t}\alpha_i\rho_i + \nabla\cdot\alpha_i\rho_i\boldsymbol{u_i} = 0 \tag{1}$$

Momentum equation for gas phase:

$$\frac{\partial}{\partial t}\alpha_g\rho_g\boldsymbol{u_g} + \nabla\cdot\alpha_g\rho_g\boldsymbol{u_g}\boldsymbol{u_g} = -\alpha_g\nabla p + \alpha_g\rho_g\boldsymbol{g} + \nabla\cdot\tau_g + F_{int,gs} \tag{2}$$

Momentum equation for solid phase:

$$\frac{\partial}{\partial t}\alpha_s\rho_s\boldsymbol{u_s} + \nabla\cdot\alpha_s\rho_s\boldsymbol{u_s}\boldsymbol{u_s} = -\alpha_s\nabla p + \alpha_s\rho_s\boldsymbol{g} + \nabla\cdot\tau_s - F_{int,gs} \tag{3}$$

τ_g is modelled as,

$$\tau_g = \alpha_g\mu_g\left(\nabla\boldsymbol{u_g} + \left(\nabla\boldsymbol{u_g}\right)^T - \tfrac{2}{3}\nabla\cdot\boldsymbol{u_g}\right) \tag{4}$$

In this study, the interphase momentum transfer, $F_{int,gs}$, is modelled using the drag correlation proposed by Arastoopour *et al.* (1990).

$$F_{int,gs} = \left(\frac{17.3}{Re_s} + 0.336\right)\frac{\rho_s}{d_s}\left|\boldsymbol{u_s} - \boldsymbol{u_g}\right|\alpha_s\alpha_g^{-2.8}\left(\boldsymbol{u_s} - \boldsymbol{u_g}\right) \tag{5}$$

Granular stress, τ_s, is modelled as,

$$\tau_s = -p_s + \mu_s\left(\nabla\boldsymbol{u_s} + (\nabla\boldsymbol{u_s})^T + \left(\mu_{b,s} - \tfrac{2}{3}\right)\nabla\cdot\boldsymbol{u_s}\right) \tag{6}$$

Granular Stress Model

Solid stress is modelled using the KTGF theory. This theory enables us to determine the fluid properties of the particle phase by accounting of the inelasticity of the particles. It assumes the solid viscosity and stress to be function of granular temperature. Granular temperature,

θ_s, is defined based on fluctuations in solid phase velocity, $\boldsymbol{c_s}$ as:

$$\theta_s = \frac{1}{3} < \boldsymbol{c_s c_s} > \quad (7)$$

KTGF introduces a transport equation for granular temperature which is given as,

$$\frac{3}{2}\left[\frac{\partial}{\partial t}\alpha_s\rho_s\theta_s + \nabla\cdot\alpha_s\rho_s\theta_s\boldsymbol{u_s}\right] = \nabla\cdot k_s\nabla\theta_s + \tau_{s,k}:\nabla u_s - \gamma_s - J_s \quad (8)$$

First term on the right hand side of this equation is diffusion of fluctuating energy along gradients in granular temperature. The second term on the right hand side is generation of fluctuating energy due to shear in the particle phase. Third term, γ_s, represents the dissipation due to inelastic collisions and the fourth term, J_s, represents the dissipation or creation of fluctuating energy because of the work done by the fluctuating force exerted by gas through the fluctuating velocity of the particles.

Granular temperature is used to estimate solid pressure, P_s, which represents the normal force due to interactions between the particles and prevents the particle phase from exceeding maximum packing limit of solids. It is modelled as given by Lun *et al.* (1984),

$$P_s = \alpha_s\rho_s\theta_s(1 + 2(1+e)\alpha_s g_o) \quad (9)$$

The solid bulk viscosity describes the resistance of the particle phase against compression. It is again modelled using the expression given by Lun *et al.* (1984),

$$\mu_{b,s} = \frac{4}{3}\alpha_s^2\rho_s g_o d_s(1+e)\sqrt{\frac{\theta_s}{\pi}} \quad (10)$$

Soild shear viscosity, μ_s, is used to calculate the tangential forces due to translational and collisional interaction of particles. In this study we use the form given by Syamlal *et al.* (1993),

$$\mu_s = \frac{4}{5}\alpha_s^2\rho_s g_o d_s(1+e)\sqrt{\frac{\theta_s}{\pi}} + \frac{\alpha_s\rho_s d_s\sqrt{\pi\theta_s}}{6(3-e)}\left[\frac{1+\frac{2}{5}\alpha_s}{(1+e)(3e-1)g_o}\right] \quad (11)$$

Similarly, the solid thermal conductivity, k_s, consists of a kinetic contribution and a collisional component. The form used in this study was proposed by Syamlal *et al.* (1993),

$$k_s = \frac{15\alpha_s\rho_s d_s\sqrt{\pi\theta_s}}{4(41-33e)}\left[1 + \frac{12}{5}\alpha_s e^2(4e-3)g_o + \frac{16}{15\pi}\alpha_s e(41-33e)g_o\right] \quad (12)$$

The dissipation of granular energy (fluctuating energy), γ_s, due to inelastic particle - particle collisions is modelled in this study as in Lun *et al.* (1984). Their work omitted the term accounting for $\nabla\cdot\boldsymbol{u_s}$ which was included in the form proposed by Jenkins *et al.* (1983).

$$\gamma_s = 12(1-e^2)\frac{\alpha_s^2\rho_s g_o}{d_s\sqrt{\pi}}\theta_s^{3/2} \quad (13)$$

The production or dissipation of granular energy, J_s, due to fluctuating force exerted by gas has two terms: first one due to correlation between particle velocity fluctuations and second due to correlation between particle and gas velocity fluctuations. Gidaspow (1994) proposes it to be modelled as, $3A_{int,gs}\theta_s$. The second term is modelled using the form proposed by Louge *et al.* (1991). The originally proposed form is divided by the radial distributional function to ensure it tends to zero as particle volume fraction approaches the maximum solid packing.

$$J_s = A_{int,gs}\left[3\theta_s - \frac{A_{int,gs}d_s(\boldsymbol{u_g}-\boldsymbol{u_s})^2}{4\alpha_s\rho_s g_o\sqrt{\pi\theta_s}}\right] \quad (14)$$

Radial distribution function, g_o, is an estimate of particle pair density at a distance equivalent to the particle diameter. It increases with increasing particle volume fraction. In this study, we used the expression by Ding *et al.* (1990),

$$g_o = \frac{3}{5}\left[(1-\alpha_s/\alpha_{s,max})^{1/3}\right]^{-1} \quad (15)$$

The radial distribution function is written as a Taylor series approximation at high volume fractions close to maximum packing. The expression in equation 15 was numerically blended with Taylor series expression to avoid convergence difficulties.

COMPUTATIONAL INVESTIGATION

The simulations in this work are carried out using STAR-CCM+ from CD-adapco. The code uses PC-SIMPLE (Vasquez *et al.*, 2000) for pressure – velocity coupling. In this algorithm, velocity components are solved together for phases in a segregated fashion. The pressure correction equation is based on total volume continuity. To avoid decoupling between the pressure – velocity fields, STAR-CCM+ uses Rhie-Chow algorithm (Rhie *et al.*, 1983) as demonstrated by Tandon (2008).

In this study, simulations were performed for all three gas superficial velocities for which experiments were performed (Case 1: 2.19 m/s, Case 2: 3.28 m/s and Case 3: 4.38 m/s). A 2-D computational domain with 44100 cells (90 X 490) was used. Uniform grid spacing was used in both the directions. Figure 1 shows the schematic of bed geometry.

All the simulations use second order convection scheme for volume fraction, velocity and granular temperature. Time step of 5 X 10^{-4} s was used for all the simulations. All the simulations were run for 50 s. The time averaged distributions of flow variables were computed for period of 20 – 50 s. The start time of 20 s ensures that the time averaging is performed only after the bed has reached quasi-steady state.

In this study we investigate the impact of the coefficient of restitution for particle – particle interactions, e, on the bed hydrodynamics. We used three values for e: 0.8, 0.84 and 0.9 in this study. The coefficient of restitution for particle – particle interactions reported in experiments ranged between 0.77 and 0.91.

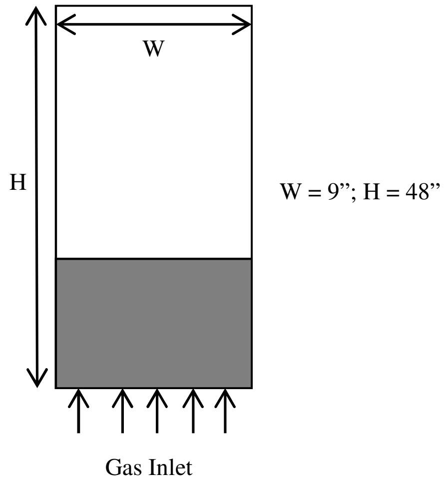


Figure 1: Schematic representation of the bed.

Boundary Conditions

Dirichlet boundary condition was used for gas phase at the inlet of the bed. Pressure outlet boundary condition was used for the top boundary. The pressure is specified as atmospheric. At the side walls, no-slip boundary condition was specified for the gas phase but it is commonly accepted in literature that it is an unrealistic condition for the particle phase in bubbling fluidized beds (Li *et al.*, 2010, Li *et al.*, 2013). In this study, we investigated both free-slip boundary conditions and the partial-slip boundary conditions proposed by Johnson *et al.* (1987) for particle phase. The equation for boundary conditions proposed by Johnson – Jackson are given by,

$$u_{s,w} = -\frac{6\alpha_s \mu_s}{\sqrt{3\theta_s}\pi\varphi\rho_s\alpha_s g_o}\frac{\partial u_{s,w}}{\partial n}, \qquad (16)$$

$$\theta_{s,w} = -\frac{k\theta_s}{\gamma_w}\frac{\partial\theta_{s,w}}{\partial n} + \frac{\sqrt{3}\pi\varphi\rho_s\alpha_s u_{s,slip}^2 g_o \theta_s^{3/2}}{6\alpha_{s,max}\gamma_w}, \qquad (17)$$

where, γ_w, is expressed in term of particle - wall restitution coefficient, e_w, as

$$\gamma_w = \frac{\sqrt{3}\pi(1-e_w^2)\alpha_s\rho_s g_o \theta_s^{3/2}}{4\alpha_{s,max}} \qquad (18)$$

The equation 17 represents the granular energy conducted to the wall after accounting for the generation of granular energy due to particle slip at the wall and the dissipation of granular energy due to inelastic collisions between the particles and the wall.

In this study, we investigate the impact of two specularity values: 0.01 and 0.05. It should be noted that free-slip condition represents specularity equal to zero.

The main parameters used in the simulations can be found in Table 1.

Parameter	Value
Gas density	1.2 kg/ m^3
Gas viscosity	1.9 X 10^{-5} Pa-s
Particle density	1131 kg/m^3
Particle diameter	3.256 mm
Particle-wall coefficient of restitution	0.92
Particle-particle coefficient of restitution	0.8, 0.84 and 0.9
Maximum packing limit	0.624
Initial bed voidage	0.424
Minimum Fluidization Velocity	1.05 m/s

Table 1: Parameters used in the numerical simulations.

RESULTS AND DISCUSSION

This section is divided into two parts, one discussing the effect of the coefficient of restitution between particle – particle collisions and second discussing the effect of the specularity coefficient.

To investigate the effect of coefficient of restitution between particle – particle collisions, simulations were performed for three values of coefficient of restitution (0.8, 0.84 and 0.9). Free-slip boundary condition was used for the particle phase at the wall in the first part.

In all the simulations it was observed that pressure dropped significantly at the inception of fluidization. The pressure drop stabilized around the mean value in all the simulations after approximately 3 seconds. The fluctuations in the pressure drop are attributed to continuous breakage and coalescence of bubbles in the fluidized bed (Taghipour *et al.*, 2005). Steady state pressure drop was measured in the experiments between z = 0.0413 m and z = 0.3048 m. It can be seen in the Figure 2 that there is no significant difference between the computationally predicted mean pressure drop for the different coefficients of restitution investigated in this study. The qualitative trend for variation in the mean pressure drop with the gas superficial velocity is in good agreement with the experiments. It is also observed that the agreement improves with an increase in the gas superficial velocity.

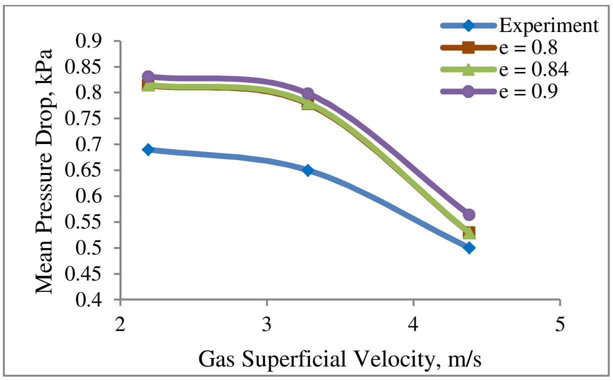


Figure 2: Comparison of the experimental and predicted mean pressure drop for three different coefficients of restitution.

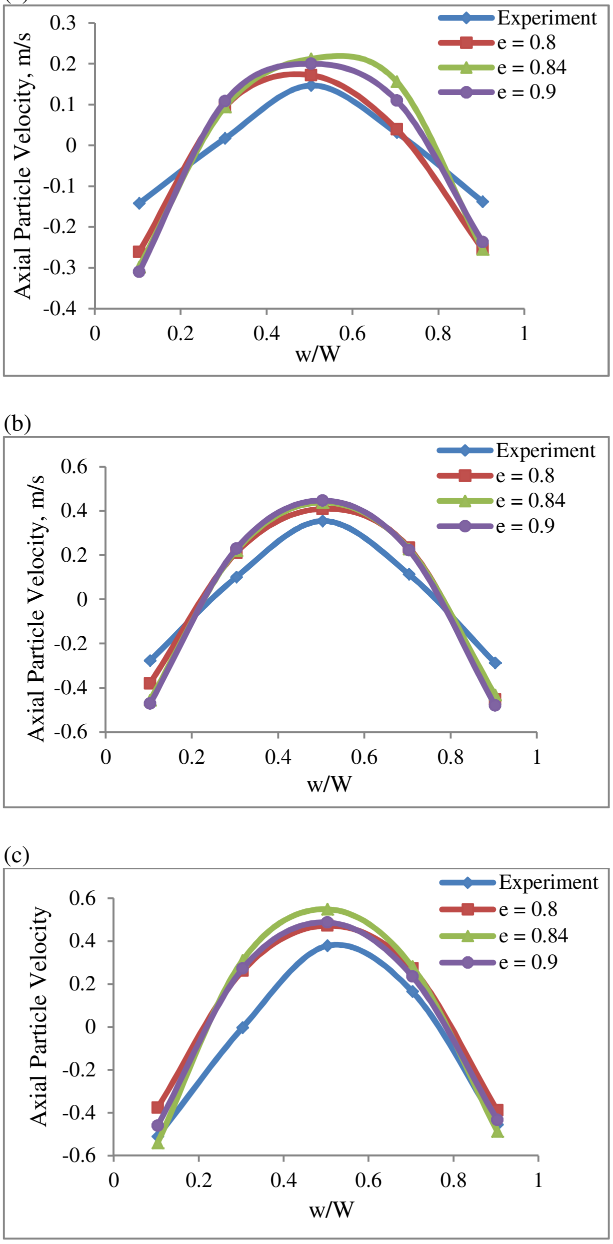


Figure 3: Axial particle velocity comparison with experimental data for three coefficients of restitution: (a) Case 1 (b) Case 2 (c) Case 3.

Particle phase velocity is one of the most important parameters in the flow pattern of a fluidized bed. Its importance is highlighted by the significance of accuracy in its prediction when investigating several phenomena such as heat and mass transfer.

The experimental measurements for the velocity profile were performed at z = 0.0762 m. The experimental time – averaged axial particle velocity is compared with the predicted simulation results for different coefficients of restitution in Figures 3 (a), (b) and (c) for $\mathbf{U}_g$ = 2.19, 3.28 and 4.38 m/s respectively. In Figure 3, w indicates the lateral location. It is observed that there is good agreement between simulation results and corresponding experimental data for the axial particle velocity. It is also seen that there is no significant impact of the coefficient of restitution on the axial particle velocity for all three cases. From Figure 3, it can be deduced that for all three gas superficial velocities, particle phase rises in the centre of the bed and falls down close to the wall indicating core – annular flow pattern of the particle phase for all cases. It is observed that with increase in rising particle velocity in the centre of the bed, downward particle velocity near the wall also increases.

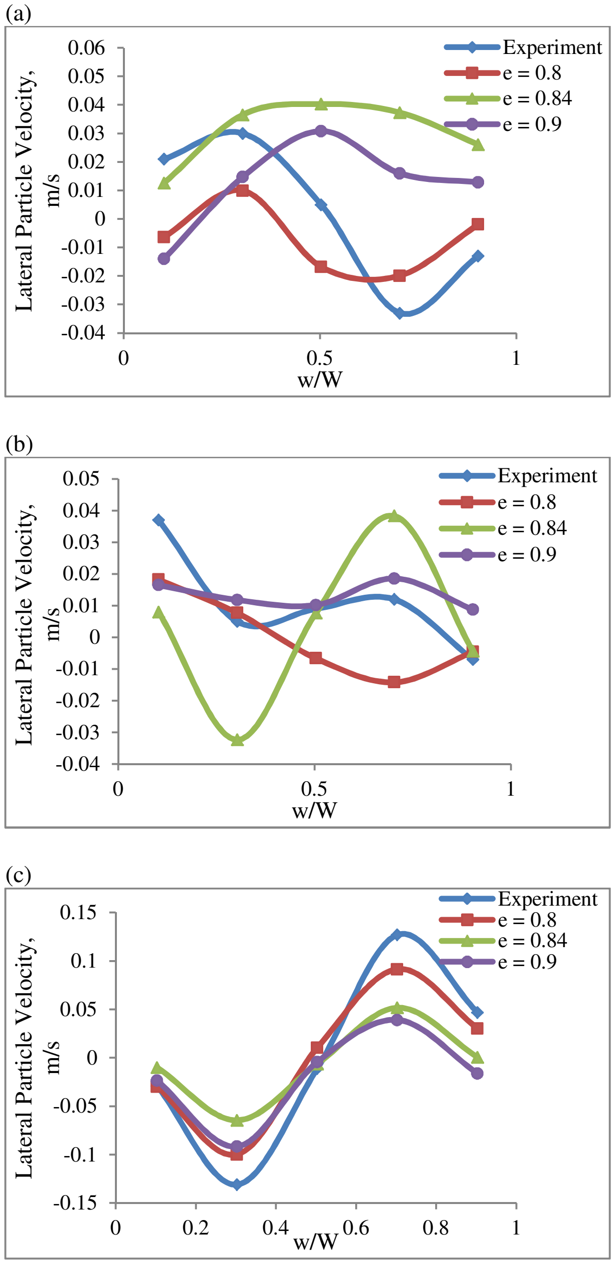


Figure 4: Lateral particle velocity comparison with experimental data for three coefficients of restitution: (a) Case 1 (b) Case 2 (c) Case 3.

Comparison between results from the simulations and the experiments for the time – averaged lateral particle velocity for different coefficients of restitution can be seen in Figures 4 (a), (b) and (c) for $\mathbf{U}_g$ = 2.19, 3.28 and 4.38 m/s respectively. It is observed that agreement for lateral particle velocity is satisfactory for the case 3 (highest gas superficial velocity). For cases 1 and 2 lateral particle velocity comparisons are less satisfactory. It can be deduced from the experimental results that solid particles are moving towards the core of the bed for case 1 and 2 at z = 0.076 m, but moving towards the wall for case 3 at z = 0.076 m. It is felt that discrepancy in cases 1 and 2 could be because of not being able to correctly capture the wall – particle interactions. So, in the second part of this study effect of specularity coefficient is investigated by employing equations from Johnson *et al.* (1987) at walls.

Specularity coefficient is indicative of the fraction of collisions which transfer momentum to the wall. It varies between zero for free-slip boundary condition and unity for perfectly diffuse collisions (no-slip boundary condition). It was first introduced by Hui *et al.* (1984). Li *et al.* (2011) demonstrated that it is closely related to local flow dynamics near the wall and the large-scale roughness of the surface.

In this study three values of specularity coefficient (0, 0.01 and 0.05) were used to investigate the effect of specularity coefficient on all the three cases. For this study we fixed the coefficient of restitution for particle – particle collisions at 0.84 and the coefficient of restitution for particle – wall collisions at 0.92. The coefficient of restitution for wall – particle interactions reported in experiments ranged between 0.90 and 0.94

It can be seen in Figure 5 that the qualitative trend for variation in the mean pressure drop with the gas superficial velocity is in good agreement with the experiments for all three values of specularity coefficient used in this study. The quantitative predictions for the mean pressure drop are similar for all the three specularity values for $\mathbf{U}_g$ = 2.19 and 3.28 m/s. The best agreement for $\mathbf{U}_g$ = 4.38 m/s is seen with the perfectly specular boundary assumption.

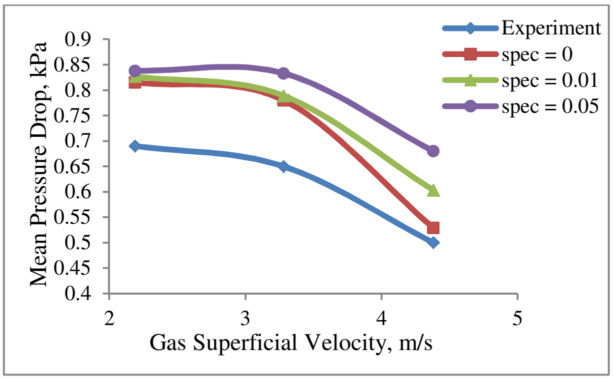
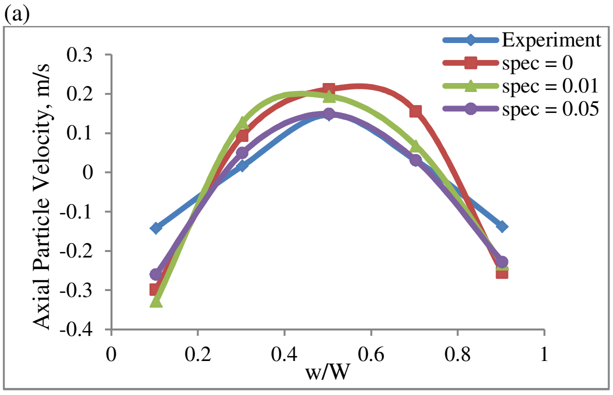


Figure 5: Comparison of the experimental and predicted mean pressure drop for three different specularity coefficients.

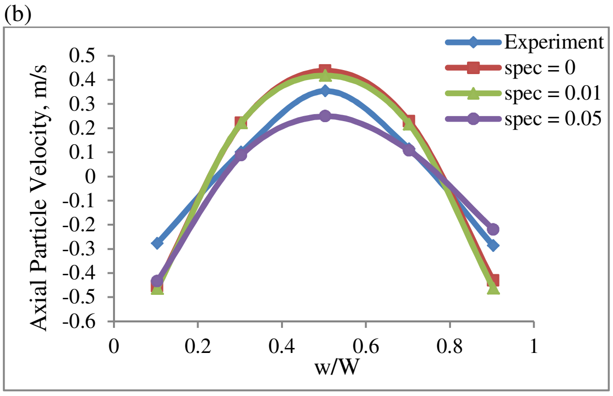
Comparison between results from the simulations and the experiments for the time – averaged axial particle velocity for different specularity coefficients can be seen in Figures 6 (a), (b) and (c) for $\mathbf{U}_g$ = 2.19, 3.28 and 4.38 m/s respectively. In general there is good agreement between simulation results and corresponding experimental data for all the three values of specularity coefficients. There is a moderate variation in the simulation results for the axial particle velocity with the specularity coefficient. The core – annular flow pattern of the particle phase is seen for all the cases. It is observed that rising particle velocity in the centre of the bed decreases with the increase in the specularity coefficient coupled with the decrease in the downward particle velocity near the wall.

The experimental time – averaged lateral particle velocity is compared with the predicted simulation results for different specularity coefficients in Figures 7 (a), (b) and (c) for $\mathbf{U}_g$ = 2.19, 3.28 and 4.38 m/s respectively. It is observed in Figure 7(a) that satisfactory agreement is seen for lateral particle velocity with the experimental results for specularity coefficient values of 0.01 and 0.05 for $\mathbf{U}_g$ = 2.19 m/s. The better agreement is seen with the value of 0.01. It is seen in Figure 7(c) that perfect specular assumption (specularity equal to zero) gives best agreement for $\mathbf{U}_g$ = 4.38 m/s. However, the comparisons for lateral particle velocity for $\mathbf{U}_g$ = 3.28 m/s are less satisfactory with only moderate qualitative agreement seen with specularity coefficient value of zero.

(a)



(b)



(c)

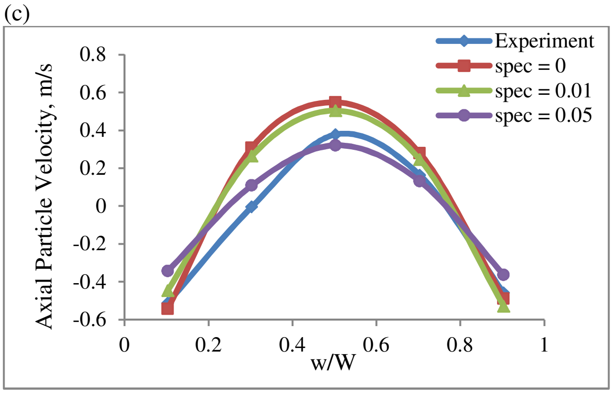


Figure 6: Axial particle velocity comparison with experimental data for three specularity coefficients: (a) Case 1 (b) Case 2 (c) Case 3.

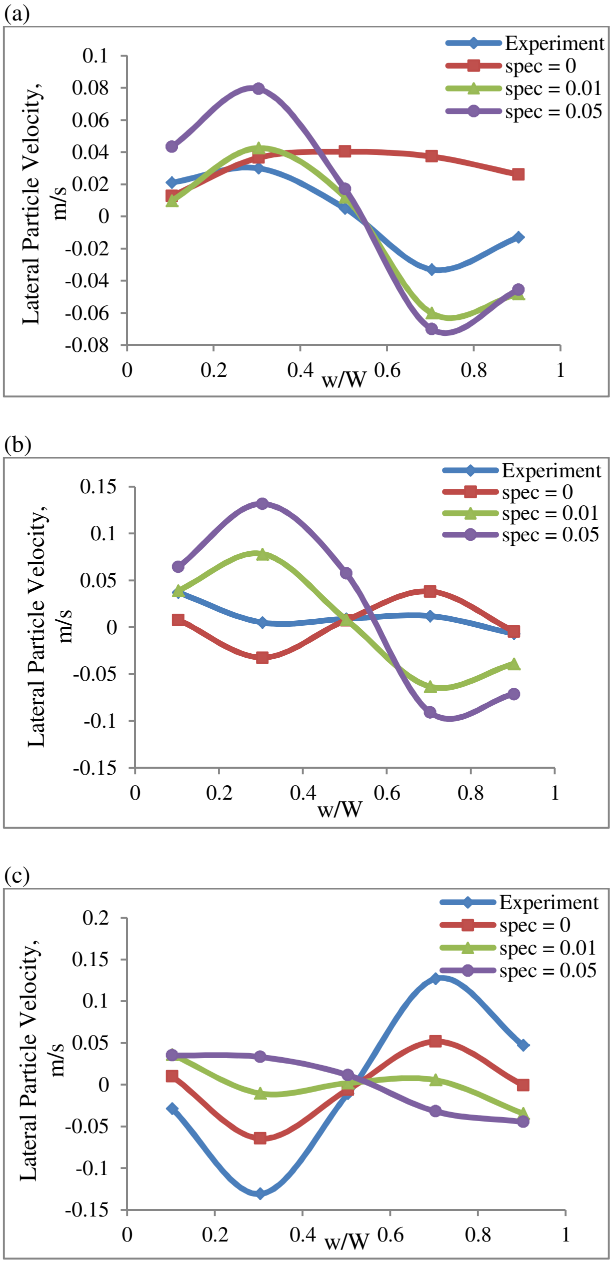


Figure 7: Lateral particle velocity comparison with experimental data for three specularity coefficients: (a) Case 1 (b) Case 2 (c) Case 3.

It can be seen from the Figure 7(a) that simulations correctly predict the particle motion towards the core of the bed for case 1 at z = 0.076 m for specularity values of 0.01 and 0.05 while Figure 7(c) shows that the simulations using specularity value of zero correctly predict the particle motion towards the wall for case 3 at z = 0.076 m. This observation is also supported by the vector plot of the time – averaged particle velocity seen in Figure 8.

The observations from Figure 7 and 8 demonstrate that the flow field (specifically lateral particle velocity) is very sensitive to the choice of specularity coefficient. This indicates that specularity coefficient will also influence the particle distribution along the lateral direction. It is also observed that the gas superficial velocity affects the specularity coefficient and that specularity coefficient decreases with increase in gas superficial velocity. This observation is consistent with the findings from other studies (Li *et al.*, 2010, Li *et al.*, 2013).

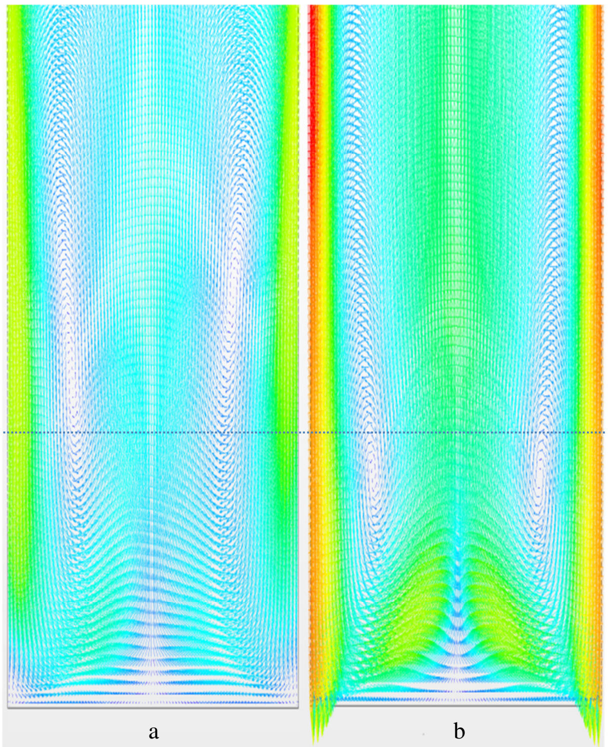


Figure 8: Vector plot of time – averaged particle velocity. (a) Case 1 (coefficient of restitution = 0.84, specularity = 0.01) (b) Case 3 (coefficient of restitution = 0.84, specularity = 0). Dotted line represents z = 0.076 m, height at which experimental velocity measurements were made.

CONCLUSIONS

Euler – Euler granular model in STAR-CCM+ based on KTGF theory was used successfully in this study to simulate the hydrodynamics of a bubbling fluidized bed using Geldart D particles. It was successful in predicting the core – annular flow pattern for solid as reported in the experiments. This study investigated two unknown model coefficients in KTGF theory: particle – particle coefficient of restitution and specularity coefficient. It was observed that the impact of the particle – particle coefficient of restitution on the hydrodynamics of the bed is not significant. However, it is shown that the specularity coefficient for particle – wall interaction has strong impact on the flow field in the bubbling fluidized bed investigated in this study. The study also demonstrates that specularity coefficient is strongly affected by the gas superficial velocity. It is felt that it will be useful to evaluate the correlation proposed for specularity coefficient by Li *et al.* (2011) for interaction between a rapid granular and a flat, frictional surface.

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