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Analysis of solid particle mixing in inclined fluidized beds using DEM simulation

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Abstract

A mathematical model has been developed to investigate the mixing behaviors of solid particles within an inclined fluidized bed, which is a system of particular interest for applications of downcomers in circulating fluidized beds. Incorporating Newton's second law of motion for calculating particle motion, the interaction among particles is successfully simulated using the discrete element method (DEM), in which the motion of fluid is modeled in a two-dimensional scheme and the motion of spherical particles is considered in a three-dimensional domain. Based on simulations, as angles of inclination are increased from 0°, 10°, 20° to 30° with respect to the vertical axis, the simulations demonstrate particle mixing phenomena with respect to fluidizing characteristics. The simulations provide a unique microscopic viewpoint of particle motion inside the bed, which cannot be observed experimentally easily. Fractional fluidization arising from distribution of gas flow along the cross-section of the bed has been found to be affected by the angle of inclination. Moreover, knowledge of microscopic mixing of solid particles, caused by circulating flow, has been explored.

Keywords: Inclined fluidized bed; Degree of mixedness; Fractional fluidization; Discrete element method

1. Introduction

Gas–solid two-phase fluidized beds are widely utilized in many physical and chemical applications including catalytic reactors, combusting boilers, drying and coating equipment owing to intensive interactions among dispersive solid particles and continuum fluidizing gas [1]. It is a well-known fact that fluidization could be determined by the balance of forces acting upon particles, which are gravitational force, gas-particle drag force and friction force among particles. Understanding of hydrodynamic behaviors is of vital importance for realistic design and reliable operation of fluidization. For the so-called dense system of which predominant portion is particles, there is limitation in clear observation of solid mixing phenomena taking place inside the equipment via experiments though there are some techniques proposed [1–4]. Consequently, numerical simulation is proposed and exploited to provide an insight into the solid mixing within fluidization [5–11].

So far, most of investigation on fluidization has been carried out using conventional straight columns. However, it is also realized that an inclined fluidized bed is a crucial part in some certain applications, such as downcomers of circulating fluidized bed combustors. Meanwhile, only a few published studies and reports are available [2,3]. Yamazaki et al. [2] are among pioneering researchers investigating the effects of inclination angle on the minimum fluidization velocity of inclined fluidized beds with various types of particles. Their experimental results presented that the pressure drop across the bed and the minimum fluidization velocity decreased with the increasing degree of inclination, leading to reduction of energy required for fluidizing solid particles inside the bed. However, their experimental investigation covers only the macroscopic behaviors of such system. To the best of our knowledge, investigation on the solid mixing based on a microscopic viewpoint has not been thoroughly reported. Therefore, numerical simulations could be considered as an alternative approach to investigate the microscopic behaviors of such inclined fluidized bed.

Recently, numerical simulation has been developed as an excellent tool to obtain microscopic information because it is not disturbed by any intrusive equipment. Many simulation

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Nomenclature

C_D	drag coefficient for a particle
d_p	particle diameter (m)
DM	degree of mixedness
f_C	contact force (N)
f_D	drag force (N)
f_G	gravitational force (N)
g	gravity acceleration ($m\,s^{-2}$)
H	height within a fluidized bed (m)
I	moment of inertia ($kg\,m^2$)
k	stiffness of spring
m	mass of a solid particle (kg)
P	pressure ($N\,m^{-2}$)
Re	Reynolds number
T_c	torque due to tangential contact force (N m)
$\bar{u}_i$	average velocity of a solid particle ($m\,s^{-1}$)
u_g	superficial gas velocity ($m\,s^{-1}$)
u_{mf}	superficial gas velocity at minimum fluidization ($m\,s^{-1}$)
v	superficial particle velocity ($m\,s^{-1}$)
V	volume a solid particle (m^3)
x_i	number fraction of particles in each sampling cells

Greek symbols

β	see Eq. (11) for definition ($kg\,m^{-3}\,s^{-1}$)
δ	displacement of a solid particle (m)
ε	void fraction
η	damping coefficient
μ	gas viscosity ($N\,s\,m^{-2}$)
μ_f	friction coefficient
ρ_g	gas density ($kg\,m^{-3}$)
ρ_p	solid particle density ($kg\,m^{-3}$)
σ_0	standard deviation for a completely segregated mixture
$\dot{\omega}$	angular acceleration (radian s^{-2})

Subscripts

g	gas phase
n	normal direction
p	solid phase
t	tangential direction

studies of gas–solid two-phase systems have been carried out using various numerical models, e.g. the two-fluid model [4–6], the discrete element method (DEM) [7–11], the hard sphere model [12] and the lattice gas cellular automation approach [13].

Yang et al. [5] have employed two-fluid CFD method with the energy-minimization multi-scale (EMMS) approach to investigate the dependence of drag coefficient on solid cluster structure within concurrent-up gas–solid flow in a riser. Their simulation indicates that the simulated solid concentration predicted by the Wen and Yu/Ergun equation is underestimated but the EMMS approach could provide the simulated outlet solid flux and voidage profile consistent with experimental results. Then, Ropelato et al. [6] also report that CFD technique with first (HIP-WIND) and second order (HIGHER UPWIND) interpolation schemes could provide simulated results of phase distribution consistent with experimental data. However, there is limitation on consideration of the interaction among each particle.

Meanwhile, with DEM technique for non-cohesive particles, Tsuji et al. [7,8] and Kawaguchi et al. [9] have pioneered simulations of key characteristics of fluidization phenomena, such as particle motion and minimum fluidization velocity, which agreed well with the experimental observations. Since then, this method has been extended to further study on behaviors of cohesive particles in fluidized beds [10]. Rhodes et al. [11] reveal that DEM method is applicable for investigating solid mixing in fluidized bed. However, only the conventional systems of vertically erected fluidized beds have been studied.

Herein, a three-dimensional model is taken into account for investigating the dependence of particle motion behavior as well as its degree of mixedness on the inclination angle of fluidized beds. To validate the developed model, simulation results are compared with the previous experimental studies [2]. Then the effects of the degree of inclination on fluidization behaviors, in particular, the pressure drop across the bed, the minimum fluidization velocity and the degree of mixedness of solid particles within the inclined bed, are comprehensively investigated.

2. Mathematical model

2.1. Assumptions

As a first step toward actual application, a simplified system of fluidization under ambient condition without chemical reaction is generally employed for investigating its hydrodynamics. In order to develop a numerical model, assumptions of the system of interest, which is equivalent to that of Yamazaki et al. [2], are set as follows:

(1) The fluid considered in this work is air at ambient condition. Therefore, it is reasonable to assume that its physical properties are constant.
(2) The fluidizing air is treated as inviscid fluid except for considering the interactions between the fluid and particles.
(3) The solid particles are spherical shape with constant density.
(4) To calculate interactions between a particle and another particle or wall, Tsuji et al. [7,8] suggest that the soft sphere model could be employed.
(5) Because of ambient condition assumption mentioned in (1) heat transfer between the particles and air as well as the particles and wall is negligible.

2.2. Motion of solid particles

To take into account the wall effects, the motion of each individual particle is modeled in a three-dimensional scheme by figuring out the Newton's second law of motion. Forces acting upon a particle are composed of the contact force (f_C), the drag force (f_D) and the gravitational force (f_G). Accordingly, the translational motion of the particle could be calculated by the following equation:

$$\dot{u} = \frac{f_C + f_D + f_G}{m} \tag{1}$$

where m is mass of the solid particle.

For rotational motion, the equation of particle motion could be given by

$$\dot{\omega} = \frac{T_c}{I} \tag{2}$$

where T_c is the torque caused by the tangential component of the contact force and I is the moment of inertia of the particle.

2.2.1. Contact forces among particles

In actual situation a particle can contact with only another particle or even the wall of the vessel. Therefore, the contact forces could be calculated using DEM technique proposed by Cundall and Strack [14]. Basically, the contact force is composed of a normal (f_{Cn}) and a tangential component (f_{Ct}), as follows:

$$f_C = f_{Cn} + f_{Ct} \tag{3}$$

$$f_{Cnij} = (-k_n\delta_{nij} - \eta_n u_{rij} n_{ij}) n_{ij} \tag{4}$$

$$f_{Ctij} = -k_t\delta_{tij} - \eta_t u_{sij} \tag{5}$$

where k is the stiffness of the spring, δ the displacement of the particle, η the damping coefficient that depends on the coefficient of restitution and the Poisson's ratio of the particle and u_{rij} is the relative velocity.

In each simulation, it is required to consider whether particle sliding exists by employing the following relation:

$$|f_{Ct}| > \mu_f |f_{Cn}| \tag{6}$$

where μ_f is the friction coefficient. In the case of sliding, the tangential contact force would be determined by

$$f_{Ct} = -\mu_f |f_{Cn}| t \tag{7}$$

2.2.2. Drag force acting on particles

The drag force is a combination between the interaction forces caused by the relative velocity between the solid particles and the fluid and the normal force due to the pressure gradient, which could be modeled as

$$f_D = \left(\frac{\beta}{(1-\varepsilon)}(v - \bar{u}) - \frac{\partial P}{\partial x} \right) V_p \tag{8}$$

where V_p is the particle volume.

2.3. Governing equations of fluid flow

Generally in numerical simulation of fluid flow, the fluid motion is considered two-dimensionally as a function of t, y and z. Locally averaged equation of continuity and Navier–Stokes equation are employed to determine the fluid motion. The SIMPLE method (semi-implicit method for pressure-linked equation) [15] and the Newton's second law of motion are employed to determine simultaneously the solutions of the fluid motion and the motion of particles. The simulation domain is represented by a set of small cells covering the whole system. It should be noted that the size of each cell must be smaller than macroscopic scale of fluidization, which could be represented by bubble size, but greater than the particles size [5,9].

In simulation, void fraction of each cell could be determined by deducting the cell volume with total volume of solid particles existing in the cell. Accordingly, the two-dimensional equation of continuity in Cartesian system is described by

$$\frac{\partial \varepsilon}{\partial t} + \frac{\partial(\varepsilon v_y)}{\partial y} + \frac{\partial(\varepsilon v_z)}{\partial z} = 0 \tag{9}$$

The equation of fluid motion is expressed as

$$\frac{\partial(\varepsilon v_i)}{\partial t} + \frac{\partial(\varepsilon v_i v_y)}{\partial y} + \frac{\partial(\varepsilon v_i v_z)}{\partial z} = -\frac{\varepsilon}{\rho_g}\left(\frac{\partial P}{\partial i}\right) + f_{pi} \tag{10}$$

The term f_{pi} in Eq. (10), representing the interaction between the particles and the fluid, could be estimated by the following equation:

$$f_{pi} = \frac{\beta}{\rho_g}(\bar{u}_i - v_i) \tag{11}$$

where $\bar{u}_i$is the average particle velocity. The β coefficient depends upon whether the system is dense or dilute. For the dense system of which the void fraction is less than 0.8, the coefficient is calculated by the well-known Ergun's equation [16]. While the void fraction is greater than 0.8, the system is dilute and the interactions between particles become weak. Therefore, the coefficient could be deduced from the Wen and Yu's equation [17] as summarized below:

$$\beta = \begin{cases} \dfrac{\mu(1-\varepsilon)}{d_p^2 \varepsilon}\{150(1-\varepsilon) + 1.75\, Re\} & (\varepsilon \le 0.8) \\ \dfrac{3}{4} C_D \dfrac{\mu(1-\varepsilon)}{d_p^2} \varepsilon^{-2.7}\, Re & (\varepsilon > 0.8) \end{cases} \tag{12}$$

$$C_D = \begin{cases} \dfrac{24(1 + 0.15\, Re^{0.687})}{Re} & (Re \le 1000) \\ 0.43 & (Re > 1000) \end{cases} \tag{13}$$

$$Re = \frac{|\bar{u} - v| \rho_g \varepsilon d_p}{\mu} \tag{14}$$

where μ, d_p and C_D are, respectively, the gas viscosity, the particle diameter and the drag coefficient for a single sphere.

3. Simulation conditions

In the present work, the geometry of the investigated inclined fluidized bed is depicted in Fig. 1. Since the height of bed is much greater than its width and depth, it is reasonably considered as a standpipe. The simulations are preformed with the angles of inclination varied from 0° to 30° with respect to the vertical axis at a step size of 10°. In an attempt to confirm the reliability of the model, the simulating results are mainly compared with the experimental results reported by Yamazaki et al. [2]. However, while it should be noted that the number of the particles equivalent to the experimental conditions is estimated to be more than

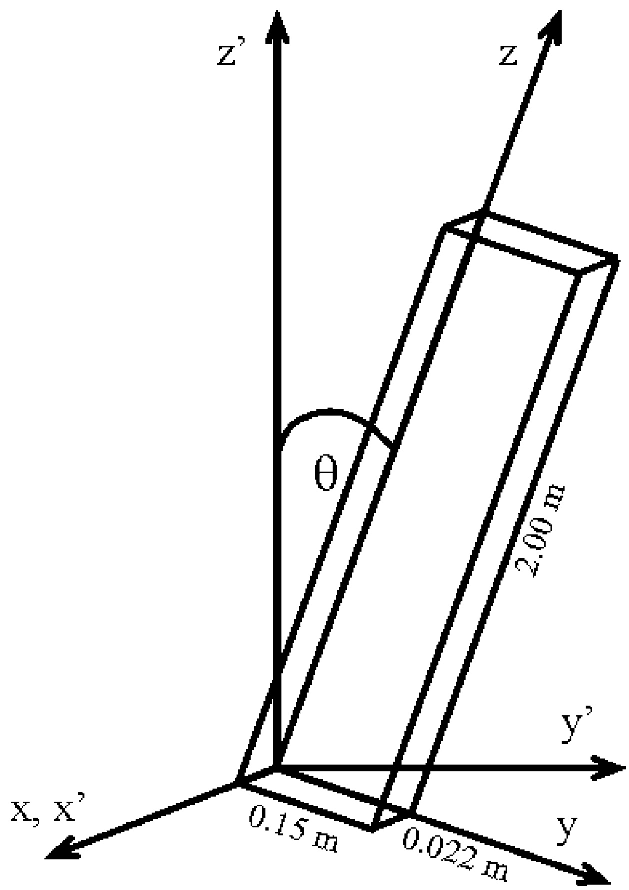


Fig. 1. Schematic drawing of the 3D inclined fluidized bed.

150,000,000, due to the restricted computational capacity, the number of the particles taken into account is limited to 20,000. Nevertheless it is still enough for representing a bed of a certain height, which could undergo fluidization [19].

According to Tsuji et al. [8] and Kawaguchi et al. [9], it has been confirmed that the coefficient of restitution and the coefficient of friction for particle–particle and particle–wall are constant at 0.9 and 0.3, respectively. Meanwhile, the time step size for calculations is a very important parameter because sufficiently small steps are required for ensuring the convergence of the simulation but it should inevitably sacrifice with relatively large computational time. For the present simulations, the time step is set to be 2×10^{-4} s, which is estimated by dividing the natural oscillation period of spring-mass system by 10 [8]. The nominal conditions of simulation are summarized in Table 1.

In each simulation, the column is set at the desired angle before allowing particles fall randomly under the gravitational influence. Then, an airflow is supplied from the bottom of the bed with a inlet velocity distributed uniformly across the whole cross-section. First, the air velocity is set to be much higher than the minimum fluidization velocity of the straightly erected column and then is gradually reduced to allow us to observe the changes in the fluidizing condition.

The wall boundary conditions are treated as slip walls, i.e. the pressure, the fluid velocity and the void fraction outside the walls are equal to those inside the wall. The outflow boundary is

Table 1
Simulation conditions

Column	
Width (m)	0.15
Height (m)	2.0
Depth (m)	0.022
Inclination angle (°)	0, 10, 20, 30
Particles	
Diameter (m)	4×10^{-3}
Density (kg/m^3)	2700
Poisson's ratio	0.25
Particle spring constant (N/m)	800
Wall spring constant (N/m)	800
Coefficient of restitution	0.9
Coefficient of friction	0.3
Number	20000
Fluid (air at ambient)	
Density (kg/m^3)	1.205
Viscosity (Pa s)	1.81×10^{-5}
Calculation parameters	
Computational domain (mm)	10×20
Time step (s)	2×10^{-4}

that the velocity gradient is zero while the fluid velocity across the walls is also set as zero.

4. Results and discussion

4.1. Model verification

As mentioned in the former section, characteristics of fluidization reported by Yamazaki et al. [2] are employed to verify the reliability of the developed model. Changes in the minimum fluidization velocity of fluidized beds with respect to the angle in inclination are compared with Yamazaki et al.'s experimental results while the visualization of flow phenomena is also taken into account. Fig. 2 shows the change in pressure drop across the bed with the increasing superficial air velocity, which also exhibits dependence of the minimum fluidization velocity (u_{mf}) on the angle of inclination. In this work, the superficial air velocity was gradually decreased from 4.5 down to 0 m/s in order to observe the fluidization phenomena. In the case of a vertical column, relationship between the pressure drop across the bed and the superficial air velocity is in a qualitative agreement with theoretical prediction, i.e. when the superficial air velocity becomes higher than u_{mf}, the pressure drop across the bed will become invariant. It is also found that the u_{mf} of the vertical column is approximately 2.1 m/s, which is well consistent with the value predicted by Ergun's equation [16]. In addition, comparison of Fig. 2(a) and (b) reveals that the effect of the inclination angle on the u_{mf} agrees fairly with the experimental results reported by Yamazaki et al. [2]. The u_{mf} gradually decreased from 2.1 to 1.5 m/s with the increase in the inclination angle from 0° to 30°. However, the value of the u_{mf} obtained in this work is rather different from the reported results due to the influence of bed height. Due to limitation of the calculating capability of computers, only 20,000 particles, which are

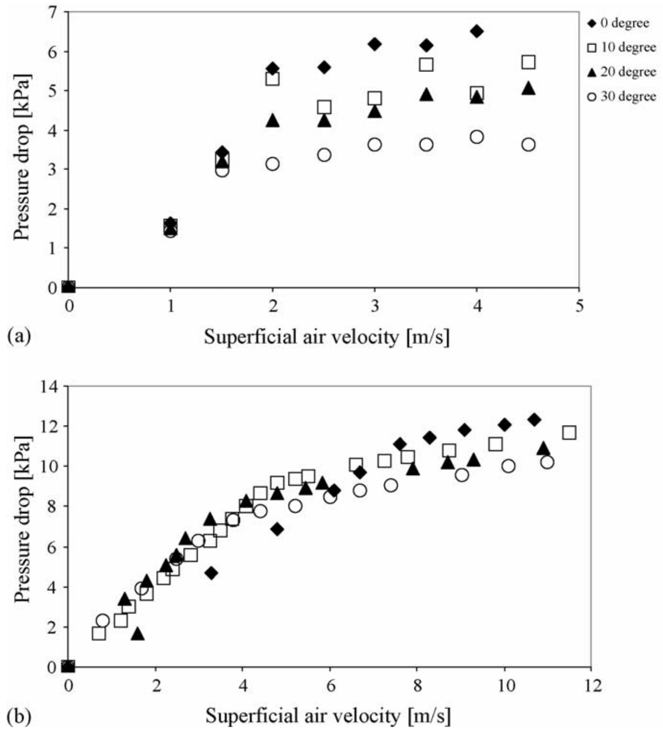


Fig. 2. Effect of angle of inclination on the minimum fluidization velocity (u_{mf}): (a) simulation results; (b) experimental results replotted from Ref. [2].

in turn equivalent to the bed height of about 40 cm, are taken into account therefore the simulating domain becomes much shallower than the bed height of Yamazaki et al.'s experiments [2].

Nevertheless, with visualization shown in Fig. 3, it could be clearly observed that formation of bubbles along the bed qualitatively resembles that of actual phenomena. With the inclination of 30°, it could be clearly seen that bubbles tend to move along the upper wall of the inclined column while the particle bed on the lower side could still undergo fluidization. With a decrease in the degree of inclination, the position of the emerging bubbles shifts to the center of the column. This is explainable that any emerging bubbles tend to penetrate through shallower particle bed because of its lower flow resistance [2–4]. Therefore, more gas bubbles would coalesce to form bigger gas slugs, which prefer to rising along the upper wall of the inclined column. Consequently, it is reasonable to consider that the developed model could acceptably simulate the actual bubbling phenomena taking place in either vertical or inclined columns. With non-uniform distribution of the emerging bubbles, turbulent movement of solid particles in the bed also becomes significantly different. These phenomena also give rise to solid particle mixing, which will be discussed in the following section.

4.2. Profile of solid particle velocity and circulation along the bed height

Since the bed depth (X axis) is much smaller than its width (Y axis) and height (Z axis), velocities of solid particles considered here are shown only in directions of Y and Z. Fig. 4(a) and (b) show a typical example of solid particle velocity distribution inside the 30°-inclined bed when the inlet air velocity is set at 4.0 m/s. At a height close to the gas distributor ($H = 0.09$ m), the particle velocity in Y direction is still somehow evenly distributed due to the uniform inlet flow of air. Majority of the solid particles tends to rise thus resulting in the negative value of the Y component of the particle velocity. On the other hand, at other higher positions, due to the influence of gravity, the solid particle velocity becomes unevenly distributed and points downward direction, leading to an increase in the Y component of the solid velocity.

On the contrary, the magnitude of the Z component of the solid particle velocity becomes much larger with slightly different distribution. It is attributable that solid particles naturally tend to entrain with air moving upward through the region with lower resistance [1,3]. Therefore, at the height of 0.09 m above the distributor, the Z component of the particle velocity becomes significantly positive, especially when the particles move close to the column upper wall. It could be seen that some portions of solid particles are dragged upward by the airflow while some particles fall down due to the gravitational and frictional effects. However, when one observes at the height of 0.49 and 0.69 m above the air distributor, the solid particle velocity becomes substantially positive because it is the region of the free surface of fluidized bed in which the solid elutriation starts to take place [1,18].

By considering both components of the particle velocity as shown in Fig. 5, the solid particles exhibit a circulating motion inside the column. It could be implied that the circulation of the solid particles takes place due to the intermingling effects of all forces acting upon the solid particles, leading to the mixing of the solid particles. Again, with incorporation of the visualized information of the solid particles one will be able to confirm that the inclination angle could provide different degree of mixing of the solid particles in the inclined fluidized bed. Therefore, it is reasonable that this unprecedented figure could be employed to elucidate the degree of mixing of solid particles inside an inclined fluidized bed.

4.3. Fractional fluidizing phenomena

Since the inclination of the column could give rise to asymmetric plane of repose along the cross-section of the column, effect of the air inlet exerting on the solid particles also changes. Typical results of simulation for a 10°-inclined column with the superficial air velocity of 4.0 m/s are shown in Fig. 6. The Z' (naturally vertical) component of air velocity, which could be determined from combination of Y and Z components of the simulation domain (Fig. 7 inset), changes insignificantly with respect to the vertical distance. Therefore, with regard to the velocity gradient, it is notable that at the lower Y position close to the upper wall of the column the local air velocity is remarkably higher than that of the opposite side. This could lead to the circulation and mixing of the solid particles as described in the above section.

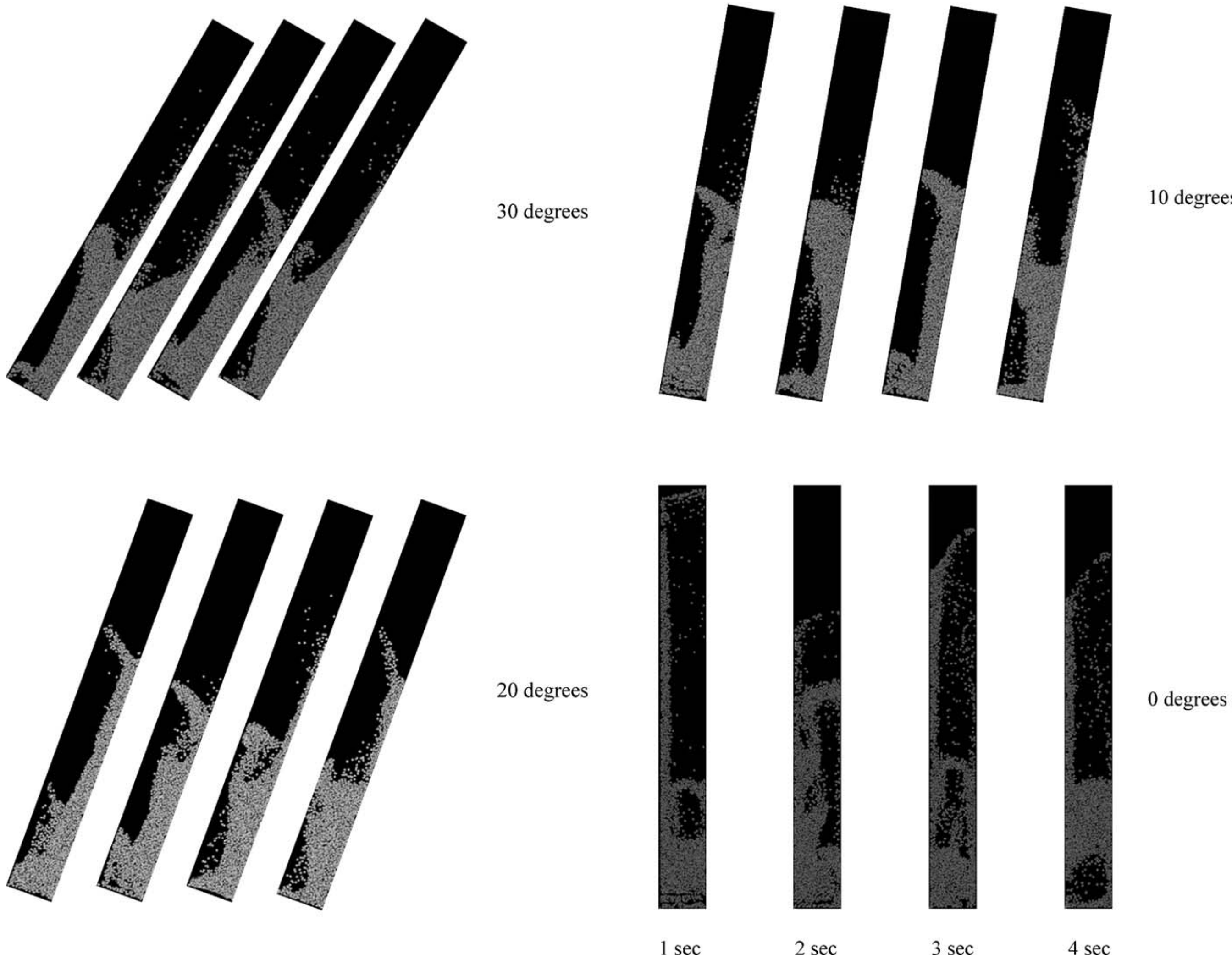


Fig. 3. Formation of bubbles inside the inclined fluidized bed at different time.

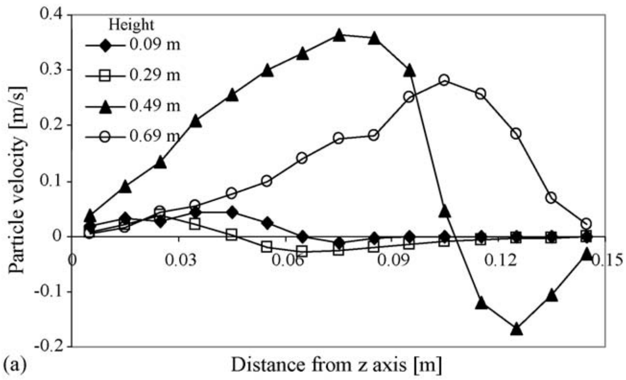
Additionally, it could be observed that the fluidization occurs partially along the cross-section of the column due to the asymmetric airflow. The solid bed with much higher thickness could exert higher flow resistance, resulting in lower local airflow. Regarding the criteria of the onset of fluidization, the fluidizing air velocity in the naturally vertical direction should be equal to the minimum fluidization velocity, u_{mf} at which the drag force exerting upon the solid particles is in a balance with the net forces of gravity and buoyancy. With this criteria, it is understandable that only some portions of the particle bed in which the average vertical air velocity is equal to or higher than u_{mf} could become fluidized. Fig. 7 reveals that an increase in the angle of inclination results in a slight decrease in fraction of bed portion undergoing fluidized state. When the faster air inlet is supplied into the column, most of the air tends to pass through the shallower region, leading to insufficient drag forces to overcome the bed resistance in the remaining region. Therefore it is reasonable to deduce that an inclined bed would become more difficult to achieve uniform fluidization state when its degree of inclination becomes steeper.

4.4. Degree of solid particle mixing due to effect of inclination

Various mixing indices, based essentially on statistical analyses, are employed to describe the solid mixing in many different industrial processes [19,20]. Rhodes et al. [11] also reported that the degree of mixing in fluidized beds is dependent on operating parameters, i.e. particle size and density. In the present work, the degree of mixedness (DM) could be assessed by evaluating the magnitude of the sample variance defined in the following equation:

$$\mathrm{DM} = 1 - \left(\frac{\sum_{i=1}^{N} \frac{(x_i - x_c)^2}{N}}{x_c(1 - x_c)} \right)^{0.5} = 1 - \frac{\sigma_{\mathrm{p}}}{\sigma_0} \tag{15}$$

where x_i and x_c are number fraction in each sampling cells and average value of all particles, respectively. σ_0 is the standard deviation for a completely segregated mixture, and N is the number of the sampling cells in the system of interest.



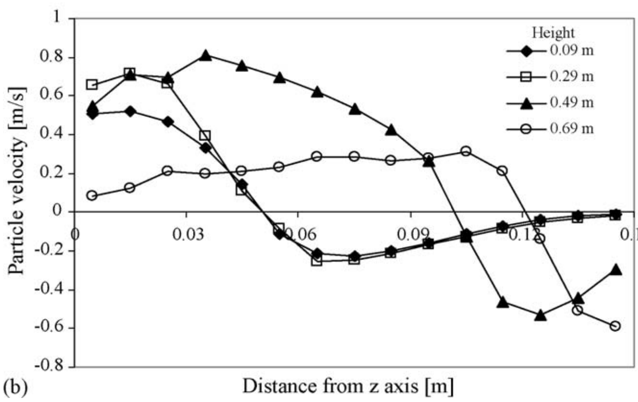


Fig. 4. Distribution of solid particle velocity inside the 30°-inclined bed with the superficial air velocity of 4.0 m/s: (a) Y component; (b) Z component.

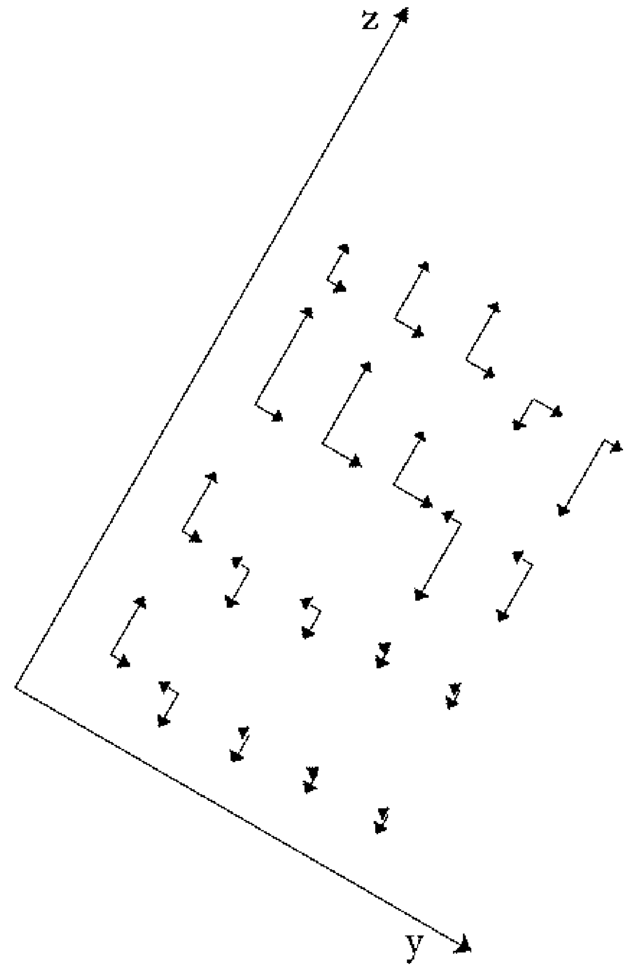


Fig. 5. Schematic diagram of particle circulating phenomenon inside the fluidized bed.

When the spatial variation of solid particles in the simulation domain has the variance equal to σ_0^2, it could be inferred that the mixing state is completely segregated. On the contrary, provided that DM is equal to unity, the solid particles could be deduced that the mixture is fully random.

In an attempt to investigate the quality of solid mixing, the solid particles in the bed were classified into two groups as shown in Fig. 8. Four representative sampling boxes referred as A, B, C and D rectangles were employed for tracing the particles circulating in the bed. After the airflow was supplied into the column, the mixing state was investigated by accounting the number of the solid particles moving from their initial positions into the sampling boxes with regard to Eq. (15).

Fig. 9 reveals that the angle of inclination has exerted some effects on the average degree of mixedness of the solid particles, which are fluidized by the superficial air velocity of 4.0 m/s. At the beginning, the mixing state drastically increases and then becomes stable after a certain period of mixing time. Interestingly, the degree of mixedness achieves the highest value with the 10°-inclined bed. An increase in the inclination angle to 20° and 30° leads to a qualitative decrease in the degree of mixing. This could be explained by the fact that with a steeper angle of inclination there exists a wider stagnant region in which the flow resistance becomes very high due to consolidation of solid particles overlying above the air distributor. With a lower angle of inclination, however, the circulation of solid particles would become more enhanced, leading to the increasing degree of mixing. These mixing phenomena could be successfully confirmed by the DEM simulation conducted in this work. These results suggested that the degree of inclination could exert some influence on the solid mixing in fluidized beds.

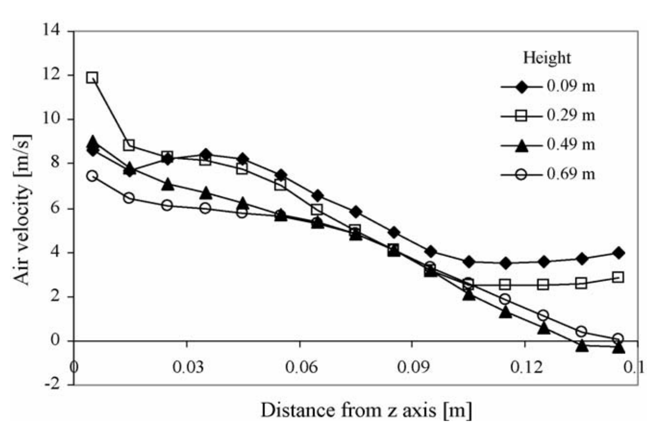


Fig. 6. Horizontal distribution of Z component of air velocity in the 10°-inclined bed with the superficial air velocity of 4.0 m/s.

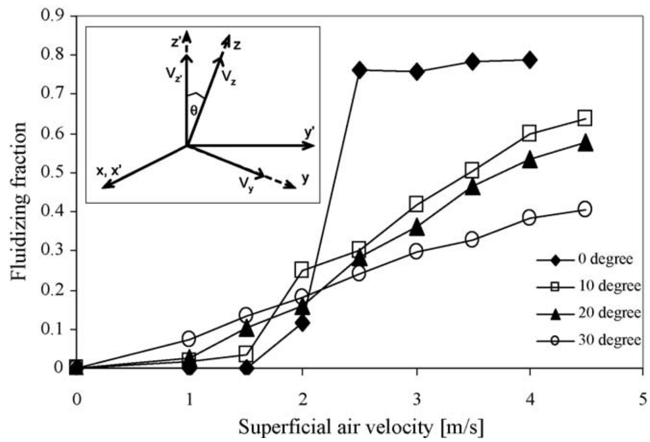


Fig. 7. Effect of angle of inclination on fluidizing fraction in the fluidized bed. The inset shows schematic diagram for considering fractional fluidization.

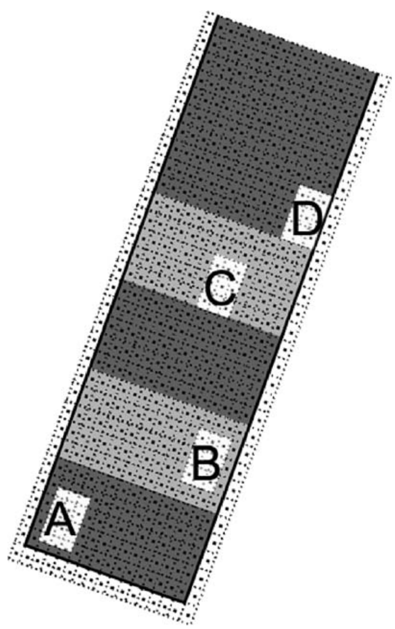


Fig. 8. Schematic diagram of tracing particles and representative sampling cells.

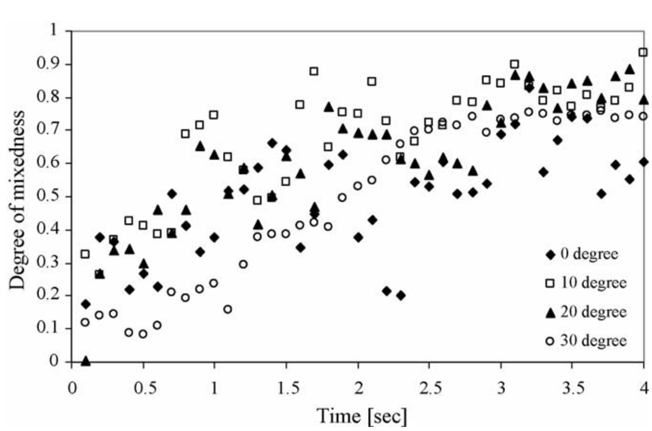


Fig. 9. Effect of angle of inclination on degree of mixedness of solid particles.

5. Conclusions

Realistic particles motion in inclined fluidized beds has successfully been simulated using the DEM technique. Comparison of the simulation with published experimental results reveals that the developed model is reliable. Not only the velocity distribution of the particles inside fluidized beds could be calculated but also the circulation phenomena, which actually takes place inside the bed but can hardly be observed experimentally, could be shown graphically. An increase in angle of inclination leads to a decrease in the fraction of the bed becoming fluidized due to the tendency of flowing air, which prefers to leave the bed through the region with the lower resistance. Finally, it is noteworthy that 10° of inclination could give rise to enhanced degree of mixedness of solid particles when compared with other inclination conditions or even the straight rising condition at the same superficial air velocity.

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