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Effect of Modeling Parameters on System Hydrodynamics of Air Reactor in Chemical Looping Combustion Using CFD Simulation

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ABSTRACT

The system hydrodynamics or flow behavior of gas and solid particles was simulated using computational fluid dynamic (CFD) model inside air reactor of chemical looping combustion (CLC). The two fluid model or Euler-Euler model was selected to use together with the kinetic theory of granular flow model (KGTF). In this study, the effect of modeling parameters including drag coefficient model, specularity coefficient and restitution coefficient between solid particles were explored. The EMMS drag model gave the highest solid volume fraction inside the system due to the particle cluster assumption in the model development. The specularity coefficient and restitution coefficient between solid particles had slightly effect on the results. In addition, the obtained results were compared with literature experiment by Shuai et al. (2012). The radial profiles of solid concentration from CFD simulation were consistent with the experimental data. The conventional core-annulus flow structure was still observed in the air reactor.

1. Introduction

Nowadays, the amount of released CO_2 into the atmosphere is the main reason for global warming problem. The recent literature shows that the circulating fluidized bed (CFB)

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technology has been widely applied in many industrial purposes. One of the applications is to use CFB technology for CO_2 capture from power generation using the chemical looping combustion (CLC) (Shuai et al., 2012). In other CO_2 capture processes, the separation of CO_2 from the N_2 requires significant energy and expense. However, CO_2 separation is easily achieved in CLC which provides a self sequestration of CO_2 stream (Mahalatkar et al., 2011a). The typical CLC is consisting of two fluidized bed reactors connecting together (Shuai et al., 2012; Samruamphianskun et al., 2012). Fuel reactor is used for providing oxygen from metal bed material for combustion reaction while air reactor is employed for reducing the metal bed material before sending them back to the fuel reactor. Generally, the metal bed material is an oxygen carrier for oxidizing or transferring oxygen in the air reactor.

For the research study about computational fluid dynamics simulation (CFD), Mahalatkar et al. (2011b) successfully studied the CFD modeling of methane combustion in fuel reactor of CLC system. The result demonstrated that CFD modeling could be an effective approach for the designing of such reactor. Their CFD model precisely predicted the trends of flue gas concentrations. For the CFD simulation of air reactor in CLC, Shuai et al. (2012) simulated CFB with cluster structure-dependent (CSD) drag coefficient model. They observed that the CSD drag coefficient model accurately predicted dynamic formation and dissolution of solid particle clusters. The derivation of this model is based on the particle cluster concept in a heterogeneous gas-solid particles flow system. Then, the model was used to predict system hydrodynamics in CLC. The contour of solid particles was dense near the wall and dilute at the center which generally called the core-annulus flow structure. Lu et al. (2011) revealed that EMMS-based drag coefficient showed good physical predictability flow behavior of both Geldart A and B in the riser. Still, in the previous literature, the suitable or optimum operating condition for simulation of air reactor in CLC reactor system was not clearly studied.

In this study, the flow behavior of gas and solid particles was investigated using CFD model inside air reactor of CLC. The main objective was to explain the obtained system hydrodynamics dynamics inside CLC system. The selected numerical model to simulate flow behavior of gas and solid particles was the two-fluid model or Euler-Euler model. This model treats each phases as fully interpenetrating continua (Cruz et al., 2006; Samruamphianskun et al., 2012). Different modeling parameters were varied to explore the effect of each parameter. The obtained CFD simulation results were validated with the experimental results published in the literature study.

2. Methodology

In this simulation, the ANSYS FLUENT 14.0 was used. The two-dimensional air reactor in CLC had 0.0762 m diameter and 6.10 m height. For two-dimensional system, the solid particles were fed from two system sides into the air reactor and flowed out at the top of the air reactor. The physical properties and simulation settings are listed in Table 1 (Shuai et al., 2011a; 2012). The solid particle was laid in Geldart A classification. Here, six drag coefficient models, four different specularity coefficients and four different solid particle-solid particle restitution coefficients were compared with the experimental results by Shuai et al. (2012).

Table 1: Parameters used in this study CFD simulation.

Description	Value
Diameter of the air reactor (m)	0.0762
Height of the air reactor (m)	6.10
Operating pressure (atm)	1
Operating temperature (K)	293.15
Gas viscosity (kg/m s)	1.85×10^{-5}
Gas density (kg/m^3)	1.20
Solid particle density (kg/m^3)	1,600
Solid particle diameter (μm)	70
Solid particle-solid particle coefficient of restitution (-)	0.97 (vary)
Wall-solid particle coefficient of restitution (-)	0.90
Specularity coefficient (-)	0.00001 (vary)
Maximum solid volume fraction (-)	0.40

The computational domain was drawn using the commercial computer aided design (CAD) program, GAMBIT (Samruamphianskun et al., 2012). The used computational domain of the air reactor in CLC had 3,500, 6,500, 9,500 and 12,500 cells as shown in Figure 1.

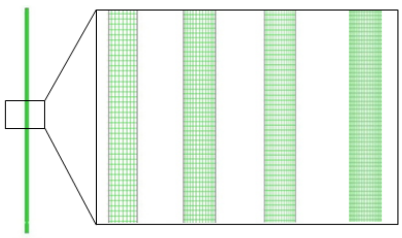

Figure 1: The computational domains of air reactor in CLC with (a) 3,500 cells, (b) 6,500 cells, (c) 9,500 cells and (d) 12,500 cells.

2.1 Mathematical model

In this study, the used numerical model of gas-solid particle two-phase flow was the

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Euler-Euler (Eulerian) model. With this model, the conservation equations of mass and momentum for the gas and solid particle phases were separately considered based on their system hydrodynamic properties. For hydrodynamics study, the energy conservation for the gas and solid phases was ignored (Shuai et al., 2011b; Chalermsinsuwan et al., 2012). The temperature of gas phase and solid particle phase then was assumed to be a constant. The conservation equations of mass, momentum and solid particle phase fluctuating energy with their constitutive equations are summarized below. In this study, the constitutive equations based on the kinetic theory of granular flow were needed to close the conservation equations.

2.1.1 Conservation equations

The mass conservation is balanced by the convective mass flux for the gas phase (g) and the solid particle phase (s):

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \nabla(\varepsilon_g \rho_g V_g) = 0 \quad (1)$$

$$\frac{\partial}{\partial t}(\varepsilon_s \rho_s) + \nabla(\varepsilon_s \rho_s V_s) = 0 \quad (2)$$

where ε is the concentration of each phase, V is the velocity, ρ is the density and t is the time. Here, the mass exchange between the phases due to chemical reaction was not considered.

The momentum conservation equation is balanced by the convective mass fluxes and the other forces such as pressure, gravity, stress tensor and momentum interphase exchange coefficient.

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g V_g) + \nabla(\varepsilon_g \rho_g V_g V_g) = -\varepsilon_g \nabla P + \nabla \tau_g + \varepsilon_g \rho_g g - \beta_{gs}(V_g - V_s) \quad (3)$$

$$\frac{\partial}{\partial t}(\varepsilon_s \rho_s V_s) + \nabla(\varepsilon_s \rho_s V_s V_s) = -\varepsilon_s \nabla P + \nabla \tau_s + \varepsilon_s \rho_s g + \beta_{gs}(V_g - V_s) \quad (4)$$

where g is the gravity acceleration, P is the pressure, β is the interphase momentum transfer coefficient or drag model and τ is the stress tensor.

The fluctuating kinetic energy conservation equation for the solid particles, as derived from the kinetic theory of granular flow (Gidaspow, 1994; Gidaspow and Jiradilok, 2009; Chalermsinsuwan et al., 2012), can be expressed as:

$$\frac{3}{2}\left[\frac{\partial}{\partial t}(\varepsilon_s \rho_s \theta) + \nabla(\varepsilon_s \rho_s \theta) V_s\right] = (-\nabla P_s I + \tau_s) : \nabla V_s + \nabla(K_s \nabla \theta) - \gamma_s \quad (5)$$

where θ is the solid fluctuating kinetic energy, K_s is the conductivity of solid fluctuating kinetic energy, I is unit vector and γ_s is the collisional dissipation of solid fluctuating kinetic energy.

2.1.2 Constitutive equations

The constitutive equations based on the kinetic theory of granular flow were needed to close the conservation equations for solving this system of equations.

The stress tensor for gas and solid particle phases are described as:

$$\tau_g = \varepsilon_g \mu_g \left[\nabla V_g + \left(\nabla V_g\right)^T\right] - \frac{2}{3}\varepsilon_g \mu_g (\nabla V_g) I \quad (6)$$

$$\tau_s = \varepsilon_s \mu_s [\nabla V_s + (\nabla V_s)^T] - \varepsilon_s \left(\xi_s - \frac{2}{3}\mu_s\right) \nabla V_s I \quad (7)$$

where μ is the viscosity of each phase and ξ_s is the bulk viscosity of solid phase.

The particle pressure can be divided into two portions. The kinetic portion describes the influence of particle translations, whereas the collisional portion accounts for the momentum transfer by direct collisions.

$$P_s = \varepsilon_s \rho_s \theta [1 + 2 g_0 \varepsilon_s (1 + e)] \quad (8)$$

where g_0 is the radial distribution function and e is the restitution coefficient between solid particles.

The shear viscosity accounts for the tangential forces. The shear viscosity of solid particles was then calculated using the formula below:

$$\mu_s = \frac{4}{5}\varepsilon_s \rho_s d_p g_0 (1 + e)\sqrt{\frac{\theta}{\pi}} + \frac{10 \rho_s d_p}{96(1 + e) g_0 \varepsilon_s}\left[1 + \frac{4}{5} g_0 \varepsilon_s (1 + e)\right]^2 \quad (9)$$

where d_p is the particle diameter.

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The bulk viscosity formulates the resistance of solid particles to comparison and expansion.

$$\xi_s = \frac{4}{3}\varepsilon_s\rho_s d_p g_0(1+e)\sqrt{\frac{\theta}{\pi}} \quad (10)$$

The radial distribution function is the probability of collisions between solid particles when they become dense:

$$g_0 = \left[1-\left(\frac{\varepsilon_s}{\varepsilon_{s,max}}\right)^{1/3}\right]^{-1} \quad (11)$$

where $\varepsilon_{s,max}$ is the volume fraction of solid phase at maximum packing condition.

The conductivity of the solid fluctuating kinetic energy specifies the diffusion of granular energy as:

$$K_s = \frac{150\rho_s d_p\sqrt{\theta\pi}}{384(1+e)g_0}\left[1+\frac{6}{5}\varepsilon_s g_0(1+e)\right]^2 + 2\rho_s{\varepsilon_s}^2 d_p(1+e)g_0\sqrt{\frac{\theta}{\pi}} \quad (12)$$

The rate of dissipation of fluctuation kinetic energy due to solid particle collision is expressed as:

$$\gamma_s = 3(1-e^2)\varepsilon_s^2\rho_s g_0\theta\left(\frac{4}{d_p}\sqrt{\frac{\theta}{\pi}}\right) \quad (13)$$

2.1.3 Drag coefficient model

In this study, the commercial ANSYS FLUENT 14.0 program with six drag or interphase exchanged coefficient models was explored. The drag coefficient model is the mathematical function which represents the dynamics of solid particles that is described by the product of the interphase momentum exchange coefficient and the slip velocity in the momentum transport equations. The high and low values of drag coefficient model imply more and less anti-translation force of solid particles inside the system, respectively. In this study, the employed drag models were Wen and Yu model, Gidaspow model, Huilin-Gidaspow model, Gibilaro model, Syamlal and O'Brien model and EMMS model (Fluent, Inc., 2011a, 2011b).

The Syamlal-O'Brien model is based on measurements of the terminal velocities of solid particles in fluidized or settling beds, with correlations that are a function of the volume fraction and relative Reynolds number (Fluent, Inc., 2011a, 2011b).

$$\beta_{gs} = \frac{3}{4}\frac{(1-\varepsilon_g)\varepsilon_g}{V_{r,s}^2 d_p}\rho_g \frac{Re_s}{V_{r,s}} C_D \left|V_g - V_s\right| \tag{14}$$

With

$$V_{r,s} = 0.5\left(A - 0.06Re_s + \sqrt{(0.06Re_s)^2 + 0.12Re_s(2B - A) + A^2}\right) \tag{15}$$

where $V_{r,s}$ is terminal velocity correlation for the solid particle phase.

$$Re_s = \frac{\varepsilon_g\left|V_g - V_s\right| d_p}{\mu_g}; C_D = \left(0.63 + \frac{4.8}{\sqrt{Re_s/V_{r,s}}}\right)^2 \tag{16}$$

$A = \varepsilon_g^{4.14}$; for$\varepsilon_g \leq 0.85$, $B = 0.8\varepsilon_g{}^{1.28}$ and for $\varepsilon_g > 0.85$, $B = \varepsilon_g{}^{2.65}$

The Wen and Yu model is appropriate for dilute system simulation (Wen and Yu, 1966).

$$\beta_{gs} = \frac{3}{4}\frac{(1-\varepsilon_g)\varepsilon_g}{d_p}\rho_g\left|V_g - V_s\right| C_{D0}\varepsilon_g^{-2.65} \tag{17},$$

where $C_D = \frac{24}{\varepsilon_g Re_s}[1 + 0.15\left(\left(1-\varepsilon_g\right)Re_s\right)^{0.687}$, $Re_s = \frac{\rho_g d_p |V_s - V_g|}{\mu_g}$

The Gidaspow model is a combination of the Wen and Yu model equation for dilute phase calculation and the Ergun equation for dense phase calculation (Gidaspow et al., 1992; Huilin et al., 2003).

For $\varepsilon_g > 0.8$:

$$\beta_{gs} = \frac{3}{4}\frac{\left(1-\varepsilon_g\right)\varepsilon_g}{d_p}\rho_g C_D \varepsilon_g{}^{-2.65}\left|V_s - V_g\right| \tag{18}$$

For $\varepsilon_g \leq 0.8$

$$\beta_{gs} = \frac{150(1-\varepsilon_g)^2\mu_g}{\varepsilon_g d_p^2} + \frac{1.75\rho_g\left(1-\varepsilon_g\right)\left|V_s - V_g\right|}{d_p} \tag{19}$$

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Huilin-Gidaspow model is also a combination of the Wen and Yu model and Ergun equation. However, the smooth switch is provided by the function when the solid volume fraction is less than 0.2. (Du et al., 2006):

$$\beta_{gs} = \Psi\beta_{gs-Ergun}| + (1-\Psi)\beta_{gs-Wen\ and\ Yu} \tag{20}$$

Where $\Psi = \frac{1}{2} + \frac{\arctan(262.5(1-\varepsilon_g)-0.2))}{\pi}$

Gibilaro model provides the continuous single compact equation over the entire range of voidages for a fluidized bed system (Du et al., 2006):

$$\beta_{gs} = \left(\frac{18}{Re} + 0.33\right)\frac{\rho_f|V_s - V_g|}{d_p}(1-\varepsilon_g)\varepsilon_g - 1.8 \tag{21}$$

with $Re = \frac{\varepsilon_g \rho_g d_p |V_s - V_g|}{\mu_g}$

The last drag model is energy minimization multi-scale (EMMS) model that develops based on the particle cluster concept. This drag model includes the effect of heterogeneous structure parameters into the momentum interphase coefficient model (Chalermsinsuwan et al, 2009; 2010).

For $\varepsilon_g \leq 0.74$:

$$\beta_{gs} = 150\frac{(1-\varepsilon_g)^2\mu_g}{\varepsilon_g d_p^2} + 1.75\frac{(1-\varepsilon_g)\rho_g|V_g - V_s|}{d_p} \tag{22}$$

For $\varepsilon_g > 0.74$:

$$\beta_{gs} = \frac{3}{4}\frac{(1-\varepsilon_g)\varepsilon_g}{d_p}\rho_g|V_g - V_s|C_{D0}\omega(\varepsilon_g) \tag{23}$$

With

$0.74 < \varepsilon_g \leq 0.82$;

$$\omega(\varepsilon_g) = -0.5769 + \frac{0.0214}{4(\varepsilon_g - 0.7463)^2 + 0.0044} \tag{24}$$

$0.82 < \varepsilon_g \leq 0.97;$

$$\omega(\varepsilon_g) = -0.0101 + \frac{0.0038}{4(\varepsilon_g - 0.7789)^2 + 0.0040} \tag{25}$$

$\varepsilon_g > 0.97;$

$$\omega(\varepsilon_g) = -31.8295 + 32.8295\varepsilon_g \tag{26}$$

3. Results and discussion

In this CFD simulation, the system hydrodynamics or flow behavior of solid particles inside air reactor of CLC was discussed and compared with experimental data by Shuai et al. (2012). In addition, the effects of various modeling parameters were discussed.

3.1 Time and grid independencies

For time independent study, the computed results showed that the solid particles in air reactor of CLC took around 20 s to fill up and came to stable or quasi-steady state condition after 50 s as shown in Figure 2. The absolute pressure was selected parameter to validate the numerical models. In this study, the results were time-averaged after 50 s and the total simulation time for each case was 70 s.

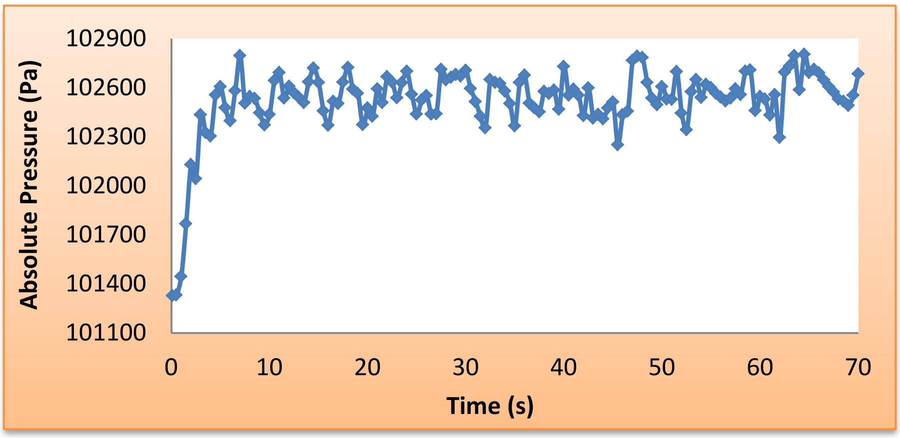


Figure 2: Time independency test by absolute pressure at 2 m height in air reactor of CLC.

For grid independent study, the simulations of air reactor with four different meshes were explored. From the results, the appropriate mesh size was found. As shown in Figure 3, the results of absolute pressure with three different meshes showed the same trend (6,500, 9,500 and 12,500 cells) but the result with 3,500 cells showed somewhat different behavior. Therefore, the 6,500 cells was selected to use in the present simulations because it gave the similar result with the higher computational domains.

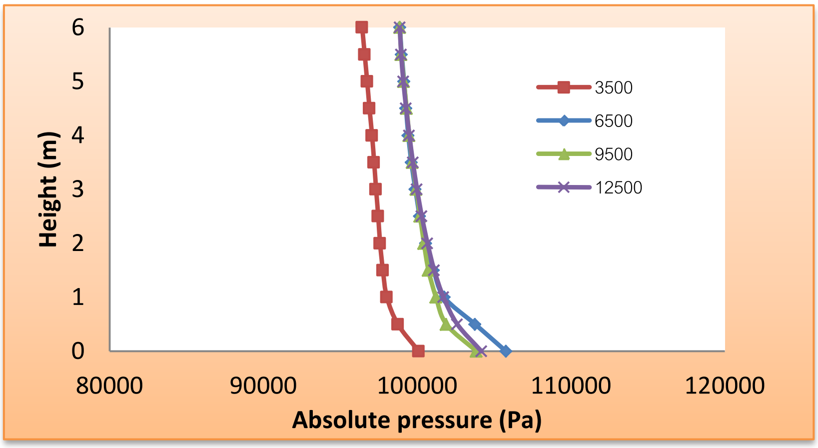
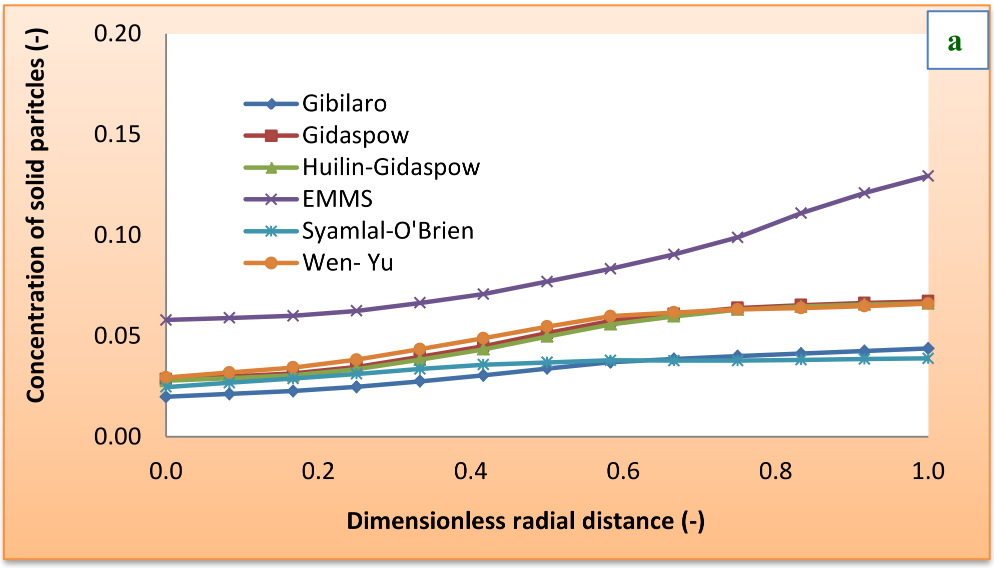


Figure 3: Grid independency test by axial absolute pressure profile in air reactor of CLC.



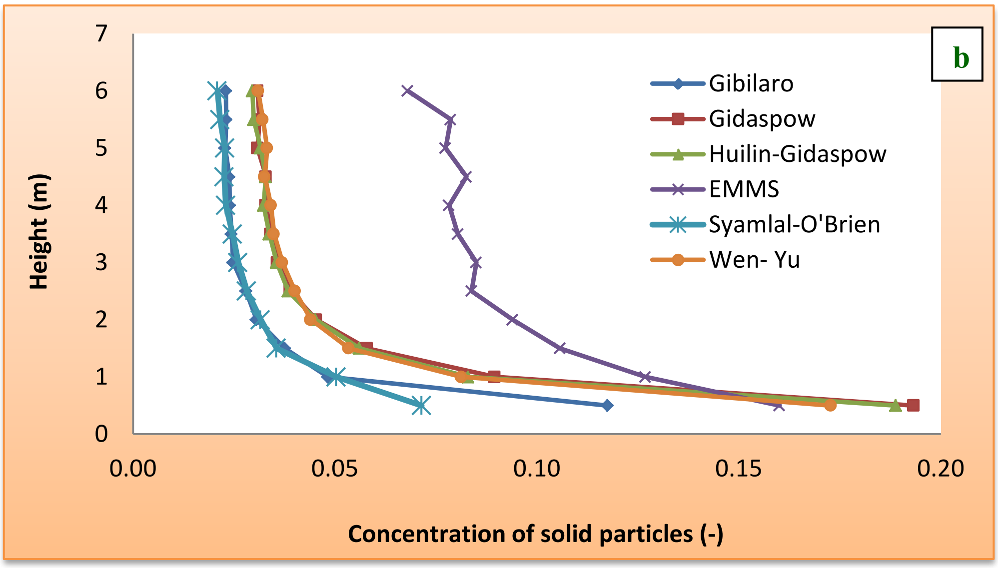


Figure 4: Effect of six drag coefficient models on concentration of solid particles for (a) radial direction at 5 m height and (b) axial direction.

3.2 Effect of drag coefficient model

Figure 4 shows the effect of six drag coefficient models on concentration of solid particles for (a) radial direction at 5 m height and (b) axial direction along the height of air reactor. From Figure 4(a), the obtained results with EMMS drag model showed higher concentration of solid particles comparing with the other drag coefficient models. The reason can be explained by the EMMS drag model is developed based on the solid particle cluster concept. The Geldart A solid particle generally agglomerates together assolid particle cluster (Chalermsinsuwan et al., 2009). The concentration profile of solid particles showed the high value near the wall region than the one at the center region which is commonly called core-annulus flow structure. From Figure 4(b), all the drag model simulations showed the high averaged concentration of solid particles at the bottom region. Then, the concentration of solid particles decreased along the height of air reactor. Again, the EMMS drag model showed higher concentration of solid particles than the other drag models.

3.3 Effect of modeling parameters

In this section, the simulations with EMMS drag model were used to compare different modeling parameters. The effect of specularity coefficient and the solid particle-solid particle restitution coefficient were explored. The other parameters were set according to Table 1. The concentration of solid particle is the factor that can be used to represent the system hydrodynamics.

3.3.1 Specularity coefficient

The specularity coefficient is the modeling parameter that describes the collision fraction of solid particles which transfer momentum to the wall. The value of specularity coefficient varies between zero and one. A value of zero means that a smooth wall is used or a free-slip boundary condition is applied at the wall and a value of one means that a rough wall is used or a partial-slip boundary condition is applied at the wall (Chalermsinsuwan et al., 2012). Chen and Wheeler (2013) reported that air velocities were very sensitive to the specularity coefficient values less than 0.10. Zhou et al. (2013) studied the effect of wall boundary condition in CFB risers. Their specularity coefficient had a pronounced influence on flow behavior when the EMMS-based drag model was used and a small specularity coefficient could result in better agreement with the experimental data.

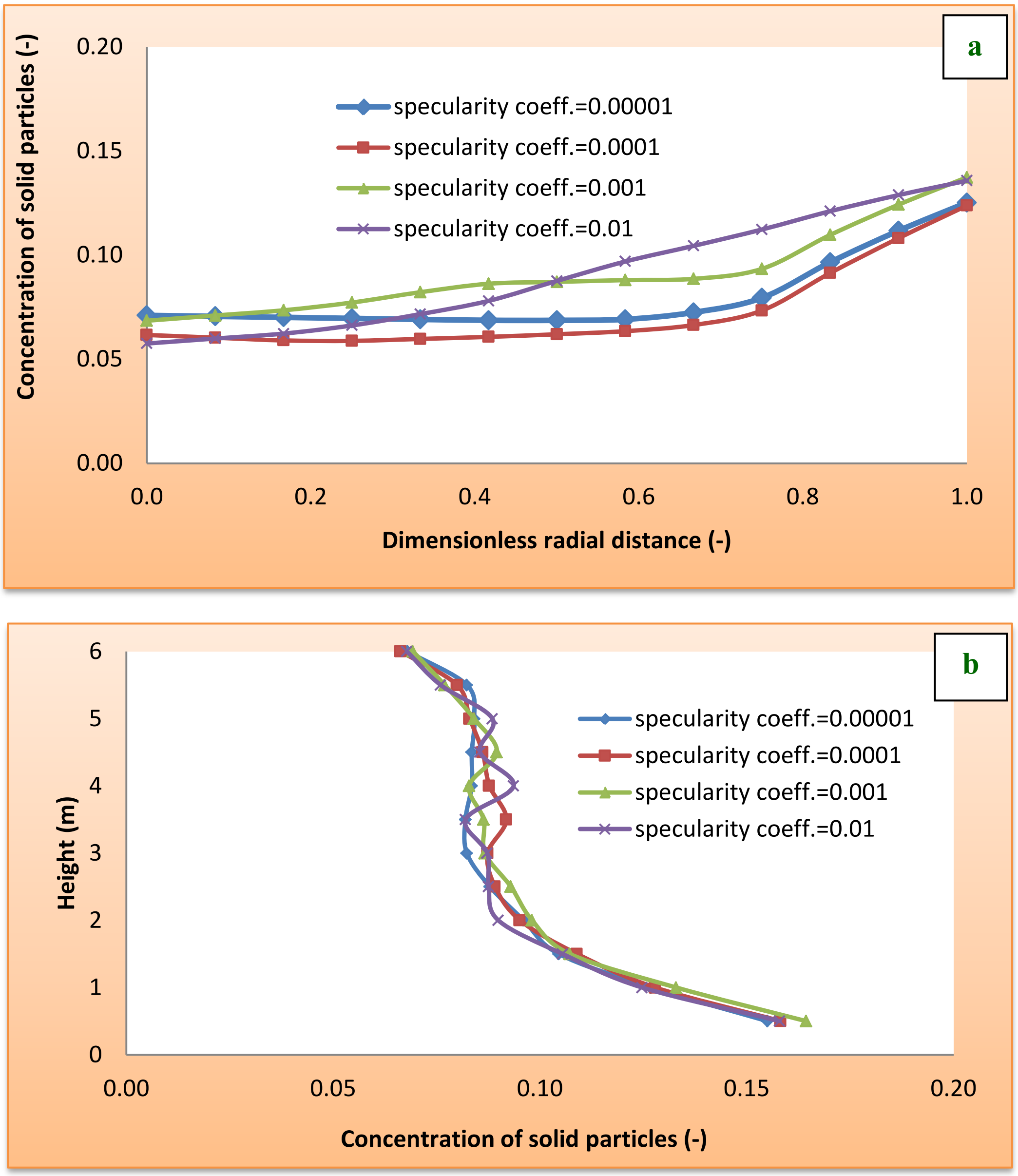
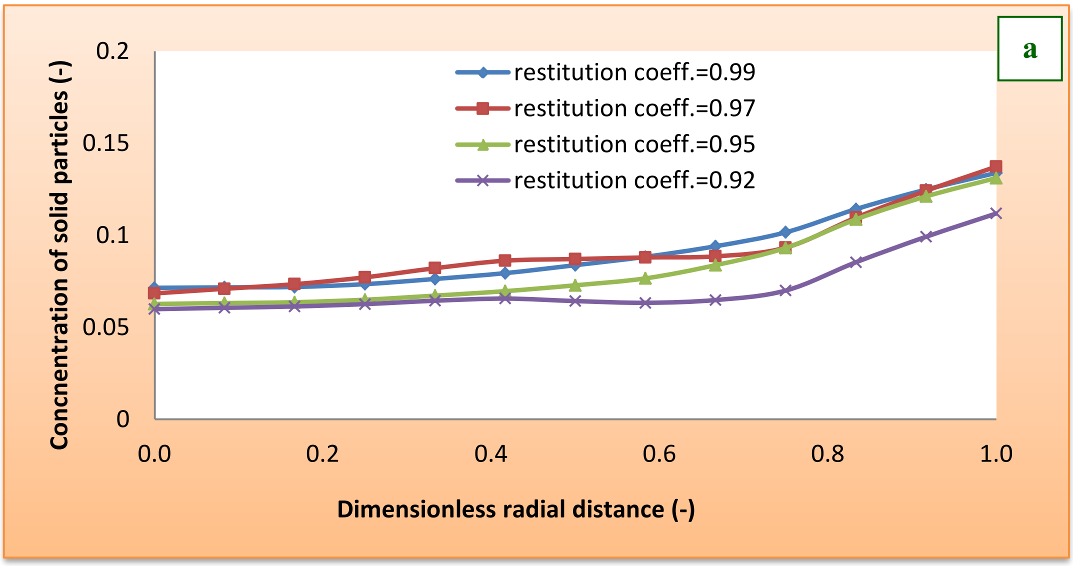


Figure 5: Effect of four specularity coefficients on concentration of solid particles for (a) radial direction at 5 m height and (b) axial direction.

Figure 5 shows the effect of four different specularity coefficients on concentration of solid particles for (a) radial direction at 5 m height and (b) axial direction along the height of air reactor. The selected specularity coefficient values were 0.00001, 0.0001, 0.001 and 0.01. At 5 m height, the system flows were already settled in fully developed condition. The effect of specularity coefficients was seen near the system wall. The high specularity coefficient value $(\varphi = 0.01)$ gave higher concentration of solid particles due to the strong friction between solid particles and wall. The low specularity coefficient value $(\varphi = 0.00001)$ means that the wall is in free-slip condition. With this condition, there is no friction between solid particles and wall. The solid particles then could freely move along the wall and had a lower concentration of solid particles. The obtained results were agreed well with Zhou et al. (2013). From Figure 5(b), all the results with different specularity coefficients had the S-shaped profiles. The concentration of solid particles was decrease along the column height. At the bottom and top of the air reactor, the concentration of solid particles was high and low, respectively. There was no significant difference in the concentration of solid particles with different specularity coefficients.



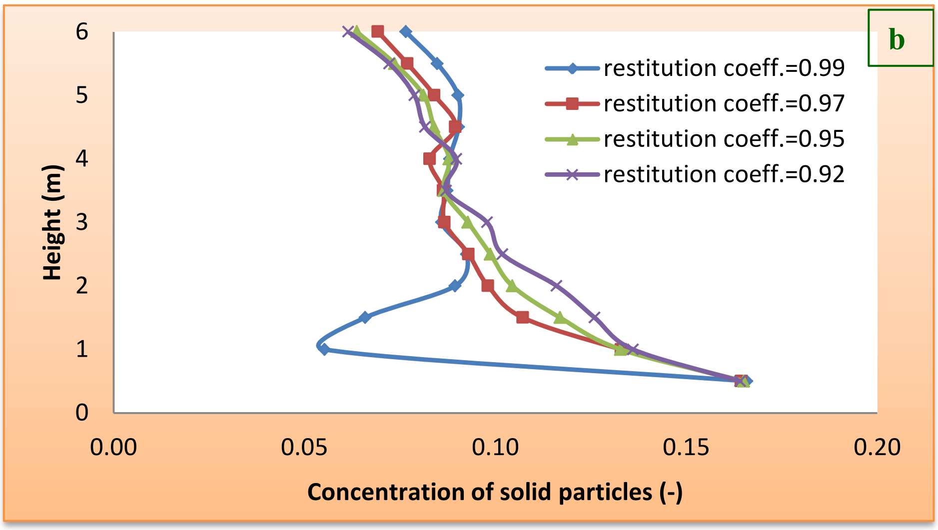


Figure 6: Effect of four solid particle-solid particle restitution coefficients on concentration of solid particles for (a) radial direction at 5 m height and (b) axial direction.

3.3.2 Restitution coefficient between solid particles

The solid particle-solid particle restitution coefficient describes the amount of the energy dissipation due to collisions between solid particles. It has an influence on the momentum conservation and granular temperature conservation of the solid particle phase (Chen and Wheeler, 2013). The restitution coefficient between solid particles also varies from a value of

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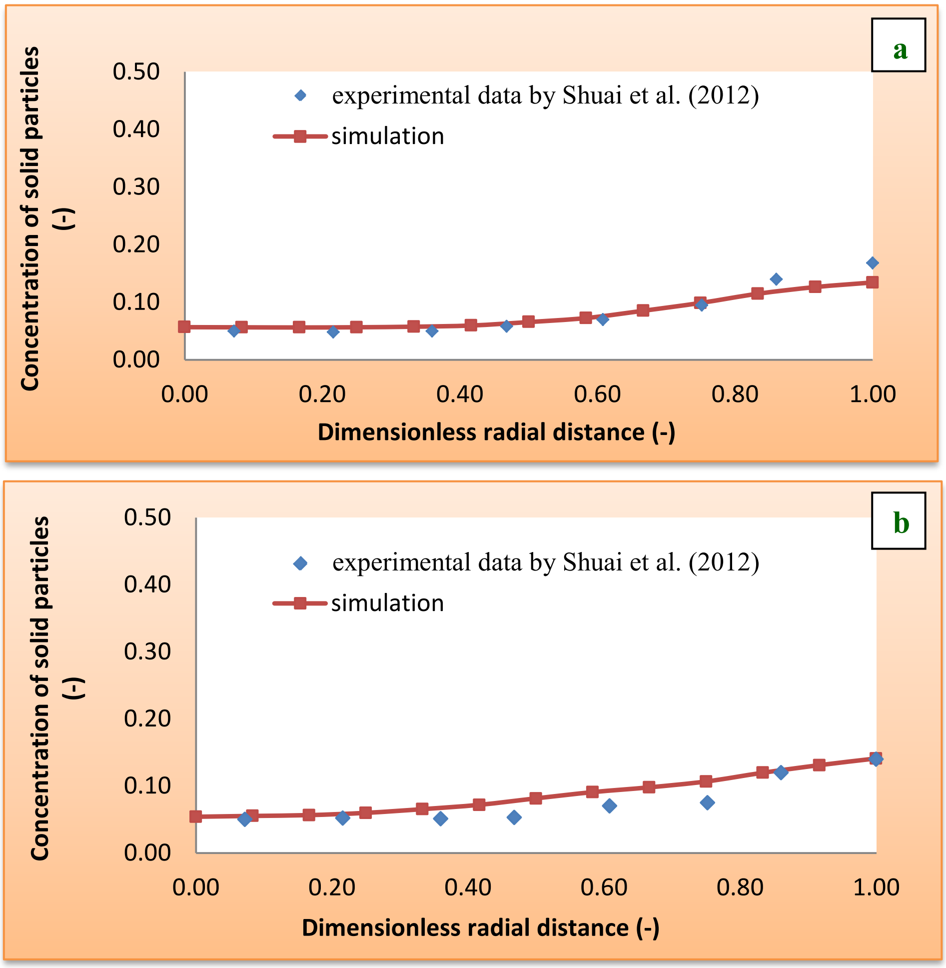

Figure 7: Distribution of solid particle concentration comparing with the experimental data by Shuai et al. (2012) at (a) 3.5 m and (b) 4.5 m heights of air reactor in CLC.

zero to one. A value of zero means that solid fluctuating kinetic energy is laid in inelastic collision while a value of one means that solid particle turbulent kinetic energy is laid in elastic collision. Chen and Wheeler (2013) examined the influence of solid particle-solid particle restitution coefficient. They noted that the free slip condition could not describe the real observed situation.

Figure 6 illustrates the effect of four different solid particle-solid particle restitution coefficients on the concentration of solid particles. The selected restitution coefficient varied among the values of 0.92, 0.95, 0.97 and 0.99. With the EMMS model and specularity coefficient value of 0.001, the overall trends of the concentration of solid particles were almost the same for different solid particle-solid particle restitution coefficient values. From Figure 6(a), the trends of all concentration of solid particles were similar that was high at the wall and low at the center. However, the high ($e = 0.99$) and low ($e = 0.92$) values of solid particle-solid particle restitution coefficient gave little higher and lower concentrations of solid particles due to the amount of elastic solid particle collision and energy loss. This explanation is confirmed in Figure 6(b) which shows high concentration of solid particles at the bottom and low at the top of the air reactor. The result supports to the experimental data by Chen and Wheeler (2013) that high value of solid particle-solid particle restitution coefficient resulted in high concentration of solid particles in the top section.

3.4 Comparison with Shuai et al. (2012) experiments

In order to compare the quantitative result with the results by Shuai et al. (2012), the result with optimum modeling condition was shown in Figure 7. The suitable condition that got closely quantitative result with the experimental data used the EMMS drag model with the specularity coefficient of 0.01 and the solid particle-solid particle restitution coefficient of 0.97. The results gave high and low concentrations of solid particles at the wall and center, respectively. The profile of concentration of solid particles was the conventional core-annulus flow structure.

4. Conclusion

This study used CFD commercial program, ANSYS FLUENT 14.0, to simulate the flow behavior of gas and solid particles in the air reactor of CLC with different modeling parameters. The drag coefficient model, specularity coefficient and solid particle-solid particle restitution coefficient were explored. The solid volume fraction result with EMMS drag model was higher than the other drag models due to the effect of solid particle cluster in model development. The specularity coefficient and restitution coefficient between solid particles had slightly effect on the results. The EMMS drag model, the specularity coefficient of 0.01 and solid particle-solid particle restitution coefficient of 0.97 gave similar result with the experiment by Shuai et al. (2012). It correctly predicted the trends of the observed radial concentration of solid particles. Then, the system hydrodynamics of solid particles was shown. All the results had the similar trend that dense solid particles were formed near the wall and dilute solid particles were occurred at the center. The simulation showed the formation of the core-annular flow structure in the air reactor (Huilin and Gidaspow, 2003).

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