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Article

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Development of computational fluid dynamics model for two initial CO₂ concentration in circulating fluidized bed reactor

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Abstract

Nowadays, the global warming is considered as a world problem because it influences the environment by increasing the average temperature of earth surface. One of the greenhouse gases that release from human activities and fossil fuels combustion in industry is CO₂. Several technologies are applied to reduce the CO₂ emission to atmosphere. In this study, the aim is to capture the CO₂ by solid sorbent adsorption with potassium carbonate supported on gamma alumina using full loop circulating fluidized bed reactor in commercial computational fluid dynamics program, ANSYS FLUENT. This study focuses on the effect of initial CO₂ concentrations from cement industry and power plant on CO₂ removal efficiency. Besides, the solid volume fraction profile is also considered. The simulation results showed the hydrodynamics in circulating fluidized bed reactor that the solid sorbent was high at the reactor wall and low at the reactor center. In addition, the independent input variables were investigated which were percentage of K₂CO₃ loading on sorbent and gas velocity. The increasing of K₂CO₃ loading on sorbent and the decreasing of gas velocity increased the CO₂ capture efficiency.

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Keywords: Circulating fluidized bed reactor; K₂CO₃ sorbent; CO₂ capture; CFD; Cement

1. Introduction

Nowadays, the world is facing climate change from excessive greenhouse gases emission into atmosphere. CO₂ is the largest share of greenhouse gases that release from several sources with human activities. The primary source comes from combustion with burning fossil fuels such as coal, oil and natural gas (electricity productions have 34%, transportations have 34% and power plants have 15% of CO₂ emission). In the other hand, non-fossil fuel combustion has 7% which has smallest share of CO₂ emission [1]. Cement industry is one of non-combustion

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Nomenclature

CO ₂	Carbon dioxide
H ₂ O	Water
K ₂ CO ₃	Potassium carbonate
k _{bw}	Reaction rate coefficient of backward reaction
k _{fw}	Reaction rate coefficient of forward reaction
KHCO ₃	Potassium bicarbonate
R	Gas constant
r _{bw}	Reaction rate of backward reaction
r _{fw}	Reaction rate of forward reaction
T	Gas temperature
ε	Solid volume fraction

sources that releasing from decomposition of carbonate (largely limestone, CaCO₃) to oxides (largely lime, CaO) and CO₂ by adding heat to the process [2].

Various technologies are developed to reduce quantities of CO₂ by separating CO₂ gas in power plants before releasing to atmosphere. There have 3 main processes to capture CO₂: (1) pre-combustion: capture CO₂ in synthesis from upstream before combustion process (2) oxy-combustion: combust with pure oxygen instead of air (composing of oxygen and nitrogen) to produce mainly CO₂ and water. Then, CO₂ is separated by condensing water. (3) post-combustion: capture CO₂ from flue gas after combustion with air. The main technologies for post combustion CO₂ capture include membrane [3], cryogenic [4], absorption [5] and adsorption [6]. Absorption with amine-based solution is applied for CO₂ capture as commercial technology in power plants. Gomes et al. [5] studied CO₂ capture by chemical absorption. Diethanol amine obtained the highest CO₂ loading capacity and the most economical among six amine-based absorbents. Blended amine solvents comprising primary (1°), secondary (2°) and tertiary (3°) amines reduced corrosive comparing with pure 1° and 2° solvents with remaining corrosive behavior [7]. Chemical adsorption with alkali-based solid sorbent is another technology for CO₂ capture system due to low price of materials. Alkali metal carbonates such as sodium carbonate (Na₂CO₃) and potassium carbonate (K₂CO₃) can react with CO₂ and water to alkali metal hydrogen carbonate [8]. In addition, energy consumption for CO₂ separation processes with K₂CO₃ was lower than monoethanolamine as the low temperature and pressure requirement [9]. Fluidized bed reactor is widely used in power plants for CO₂ capture system owing to this reactor provides a lot of advantages. For instance, fluidization has well mixing between particles and gases in reactor. It has higher gas–solid contact surface area that leads to high mass and heat transfer [10]. Furthermore, circulating fluidized bed reactor (CFBR) is developed for operating as continuous processes. For CO₂ capture, CFBR has 3 components composing of CO₂ adsorption in riser, separation between gas–solid in cyclone and sorbent regeneration in downer. Yi et al. [6] demonstrated the CO₂ removal system with continuous potassium-based sorbent circulation in a bench scale fast-fluidized bed reactor. CO₂ removal efficiency had values between 32% to 73%. The CO₂ removal increased when decreasing gas velocity and increasing solid sorbents circulation. Water vapor content was major parameter on the overall CO₂ removal. Also, Chang et al. [11] employed amine-based adsorbent in circulating fluidized bed reactor. The reaction mainly occurred in the bottom of adsorber. The velocity, solid volume fraction and gas–solid species concentration were confirmed to be the variables which affected CO₂ removal.

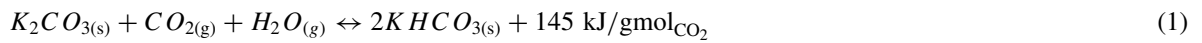
Computational fluid dynamics (CFD) uses the numerical method to analyze the transport phenomena of fluid flow. Physical properties such as velocity, pressure and density are specific parameters for implying in conservation equations consisting of mass, momentum and energy. Wang et al. [12] investigated CO₂ capture system with K₂CO₃ supported on Al₂O₃ in circulating fluidized bed reactor including an adsorber and a regenerator. Their computational fluid dynamics model used the multiscale model to represent the clustering effect that agreed better with experimental data than conventional model. It also found that CO₂ was adsorbed in dense phase more than dilute phase. Nouri et al. [13] used the potassium carbonate solid sorbent in circulating fluidized bed. The height of riser decreased from 6 m to 3 m to reduce cost of installation. Moreover, variables comprised of solid sorbent flux and steam content were operated with different inlet dry gas flows to find the same efficiency in these two circulating fluidized bed reactors.

The present study aims to demonstrate the CO₂ capture system in looping of circulating fluidized bed reactor for continuous adsorption and regeneration with K₂CO₃ supported on Al₂O₃. The predicted results are verified with the experimental results from [6]. The variables in terms of K₂CO₃ loading and gas velocity that affects CO₂ removal are investigated with CFD simulation.

2. Mathematical models

2.1. Governing equations

In this study, the Eulerian–Eulerian two-fluid flow model consists of the continuity equations, momentum conservation equations, energy conservation equations and species transport equations for gas phase and solid phase. The kinetic theory of granular flow taken from [13] is also included in the model. K₂CO₃ supported on γ -alumina is solid sorbent for CO₂ capture. The equilibrium reaction is described in Eq. (1). CO₂ reacts with K₂CO₃ and water to produce KHCO₃ which is adsorption reaction. In contrast, KHCO₃ decomposes in backward direction when temperature increases which is desorption reaction. Kinetics of forward and backward reactions are applied from [14] as shown in Eqs. (2) and (3).



$$r_{fw} = k_{fw} [CO_2]^{0.4} [H_2O]^{0.4} \varepsilon_{K_2CO_3}; k_{fw} = 1 * 10^{-10} \left[e^{\frac{70}{RT}} \right] \quad (2)$$

$$r_{bw} = k_{bw} \left(\frac{1}{[CO_2]} \right)^{0.15} \left(\frac{1}{[H_2O]} \right)^{0.15} \varepsilon_{KHCO_3}; k_{bw} = 7.83 * 10^{-3} \left[e^{\frac{-0.000502}{RT}} \right] \quad (3)$$

2.2. System description and boundary conditions

The simulated two-dimensional circulating fluidized bed reactor composes of an adsorber with a height of 3 m and diameter of 0.6 m, a cyclone, a regenerator with a height of 1.15 m and diameter of 0.64 m and a loop seal with a height of 0.4 m and diameter of 0.43 m as shown in Fig. 1.

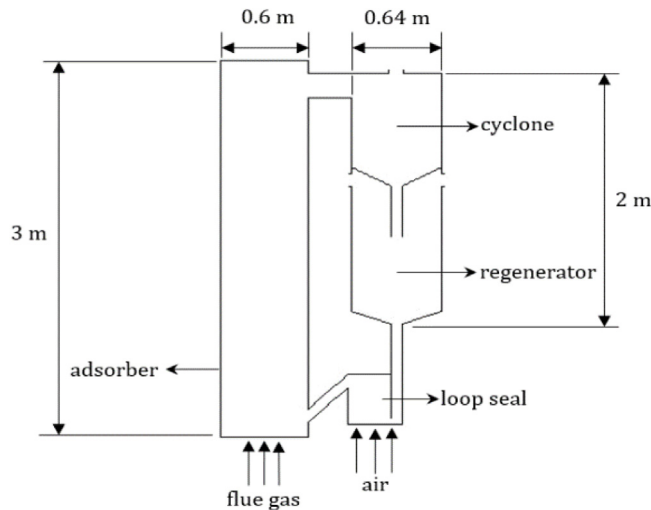


Fig. 1. Schematic drawing of circulating fluidized bed reactor.

Flue gas is fed to the bottom of adsorber while solid sorbent is packed in adsorber. CO₂ is adsorbed by solid sorbent. Then, clean gas containing nitrogen, oxygen, and water vapor leave the reactor through outlets of top of the regenerator zone. Rich solid sorbent is regenerated by temperature and exhaust CO₂ leaves the reactor at two sides of regenerator zone. The regenerated solid sorbent then passes through a loop seal to an adsorber. Air is fed at bottom

Table 1. Parameters used in the simulation.

Simulation parameters	Value	Unit
Particle density	1530	kg/m ³
Particle diameter	75	μm
Inlet gas velocity (adsorber/regenerator)	2/0.1	m/s
Inlet gas temperature (adsorber/regenerator)	343.15/423.15	K
Inlet gas species mass fraction (adsorber/regenerator)	CO ₂ = 0.225/0, H ₂ O = 0.092/0, O ₂ = 0.161/0.23, N ₂ = 0.522/0.77	–
Initial solid temperature	343.15	K
Initial solid volume fraction	0.50	–
Time step	0.001	s

of a loop seal to circulate solid sorbent as continuous fluidized bed system. The detailed operating parameters in the simulation are summarized in [12] and listed in Table 1.

For time independency test, the model is simulated for 250 s. The results indicated the quasi-steady state since 240 s. The results of the last 10 s were then calculated as time-averaged values.

2.3. Simulation method

To investigate the effect of independent variables on CO₂ removal, an experimental is designed using a two-level factorial design. This methodology helps experimenter to design the simulation with least simulation cases. The two factors are K₂CO₃ loading at 0.128 and 0.5 and gas velocity at 1.5 m/s and 3.0 m/s. The response variable for this system is CO₂ removal efficiency.

3. Results and discussion

3.1. Mesh independency test

In order to obtain accuracy results, mesh independence was performed with four values of quadrilateral computational mesh as shown in Fig. 2(a), consisting of 10 000, 15 000, 20 000 and 25 000 elements. By comparisons of absolute pressure at the middle of regenerator zone, the mesh with 20 000 elements predicted the value with only small deviation comparing to the higher elements. Therefore, mesh with 20 000 elements was chosen to obtain the accurate solution.

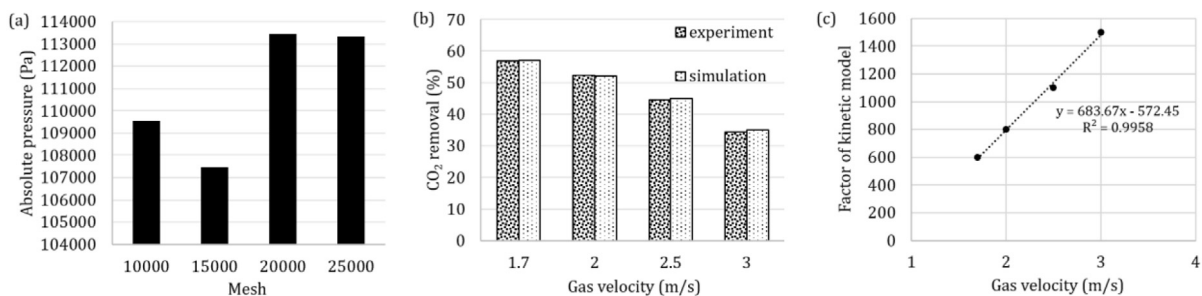


Fig. 2. (a) Absolute pressure in regenerator for four sets of mesh, (b) CO₂ removal efficiency for different gas velocity and (c) relationship between gas velocity and factor of kinetic model.

3.2. Model validation

To validate the model, the CO₂ removal efficiency in this simulation was compared with experimental data from [6] as shown in Fig. 2(b). The data derived from this kinetics model did not agree well with the experimental CO₂ removal data because different adsorbent was used. The kinetics model from [14] used sodium carbonate (Na₂CO₃)

as solid sorbent. In addition, the different system size was performed that caused the changing in mass transfer and reaction rate. Thus, the factors of kinetics model were adjusted to consistent with the experimental data that were 600, 800, 1100 and 1500 for gas velocities at 1.7, 2.0, 2.5 and 3.0, respectively. After that, the linear relationship between factor and gas velocity are shown in Fig. 2(c). The predicted CO₂ removal data by the presented model with adjusting factors of kinetic model agreed well with the experimental data. This model was then used in other simulation cases.

3.3. System hydrodynamics

Since there is no hydrodynamics experimental result to validate with the simulation results, then Fig. 3 is compared with the fluidization theory. Fig. 3(a) displayed the aggregation of solid especially near the wall due to no slip velocity boundary condition and low quantities at center of adsorber. Also, the solid volume fraction in riser and regenerator was low and high, respectively. Fig. 3(b) shows that the solid decreased along reactor height that represented fast fluidized bed in adsorber. In the other hand, solid volume fraction in regenerator had bubble with negligible deviation that was the hydrodynamics of bubbling fluidized bed regime.

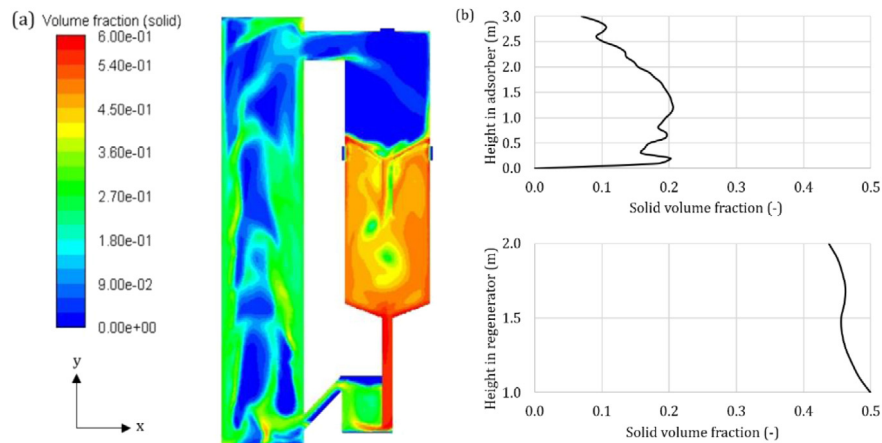


Fig. 3. (a) Instantaneous profile of solid volume fraction and (b) time averaged plots of axial distributions of solid volume fraction.

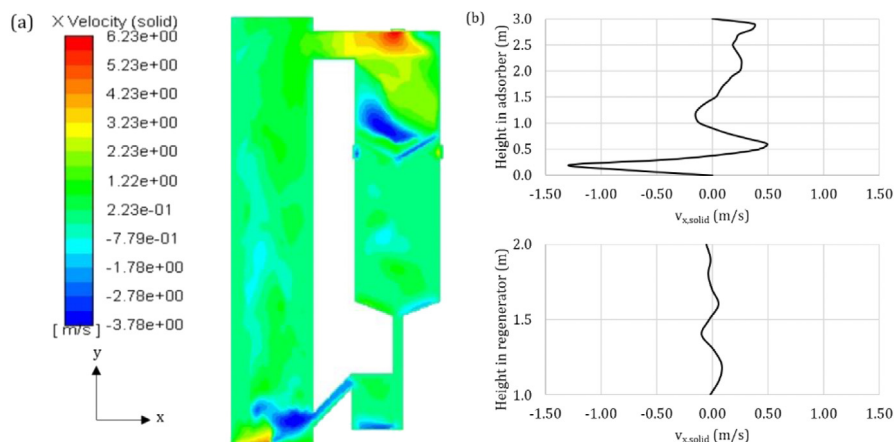


Fig. 4. (a) Instantaneous profile of solid velocity in x direction and (b) time averaged plots of axial distributions of solid velocity in x direction.

Fig. 4(a) depicts the solid velocity in x direction that shows lateral direction of fluid flow. The solid that transported from loop seal pipe had negative radial velocity. Then, the velocity had positive value according to fluctuation of solid. The decreasing of transportation area caused the velocity to fluctuate. After that, velocity slightly increased in positive direction along adsorber height to transport the solid sorbent to the regenerator. Mostly solid in the regenerator was moved down with gravity force. Thus, the radial velocity was quite constant as shown in Fig. 4(b).

Fig. 5(a) shows the solid phase axial velocity. In the center of reactor, axial velocity had the highest positive value. Then, axial velocity decreased when closing the wall. Fig. 5(b) shows distribution of solid velocity in y direction. In the adsorber, the velocity value near the wall was lower than zero from no slip velocity boundary condition and had zero value at the wall of reactor. This means that the solid flows up in the center while the solid near the reactor wall flows down. In the other hand, the regenerator had the opposite trend with adsorber and less deviation of velocity because of bubbling regime. This means that the solid flows down in the center while solid near the reactor wall slightly flows up.

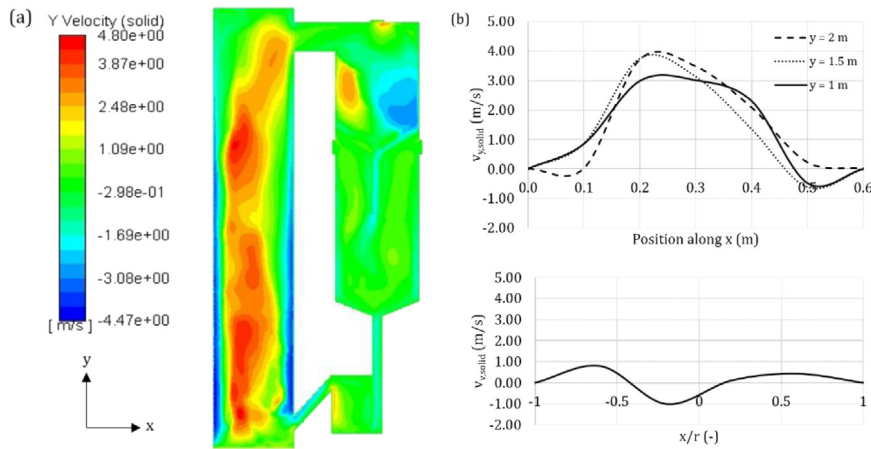


Fig. 5. (a) Instantaneous profile of solid velocity in y direction and (b) time averaged plots of radial distributions of solid velocity in y direction.

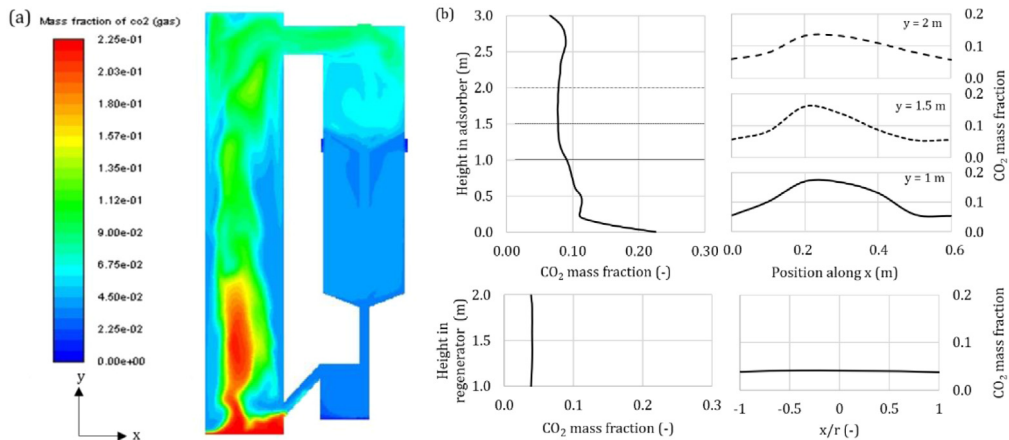


Fig. 6. (a) Instantaneous plot of CO₂ mass fraction and (b) time averaged plots of axial and radial distributions of CO₂ mass fraction.

3.4. Adsorption reaction

Fig. 6(a) shows the instantaneous profile of CO₂ mass fraction. CO₂ mass fraction was highest value at the bottom due to the gas inlet that containing CO₂. As the height of reactor increasing, CO₂ mass fraction was continuously decreased as CO₂ adsorption reaction occurred. Moreover, CO₂ desorption in regenerator was occurred throughout the reactor. Thereby, the homogeneous CO₂ mass fraction in this zone was observed as can be seen in Fig. 6(b).

CO₂ capture using solid sorbent adsorption is widely performed for flue gas from post-combustion by coal. However, there still have several sources of CO₂ emission. In this study, other sources of CO₂ emission that has higher CO₂ concentration than flue gas will firstly use this technology to remove CO₂.

One source that should be concerned is gas from cement industry that has higher CO₂ concentration as shown in Table 2. Apart from the different CO₂ concentration, other components include water vapor, oxygen and nitrogen are different. CO₂ and water vapor concentration are reactant that effect to CO₂ adsorption and desorption. The water vapor concentration is shown in the adsorption–desorption reaction as displayed in Eqs. (2) and (3). For Fig. 7(a) and (b), the CO₂ in CO₂ capture process of flue gas from coal fired power plant was higher than the CO₂ in CO₂ capture process with gas from cement industry. Thus, the CO₂ concentration for CO₂ capture process of flue gas from coal fired power plant was more captured with the same solid sorbent concentration and gas velocity.

Table 2. Mole fraction from two sources.

Source	Coal fired power plant [9]	Cement industry [15]
CO ₂	0.151	0.224
O ₂	0.148	0.023
N ₂	0.550	0.681
H ₂ O	0.151	0.072

The results were then analyzed with two-level factorial design method. Fig. 8 illustrates the main effect plot of K₂CO₃ loading at 0.128 (−1) and 0.5 (+1) and gas velocity at 1.5 (−1) m/s and 3.0 (+1) m/s on CO₂ removal efficiency. Increasing of K₂CO₃ loading increased CO₂ removal because K₂CO₃ was reactant of CO₂ adsorption reaction. The high gas velocity decreased CO₂ removal because the contacting time between gas and solid was reduced.

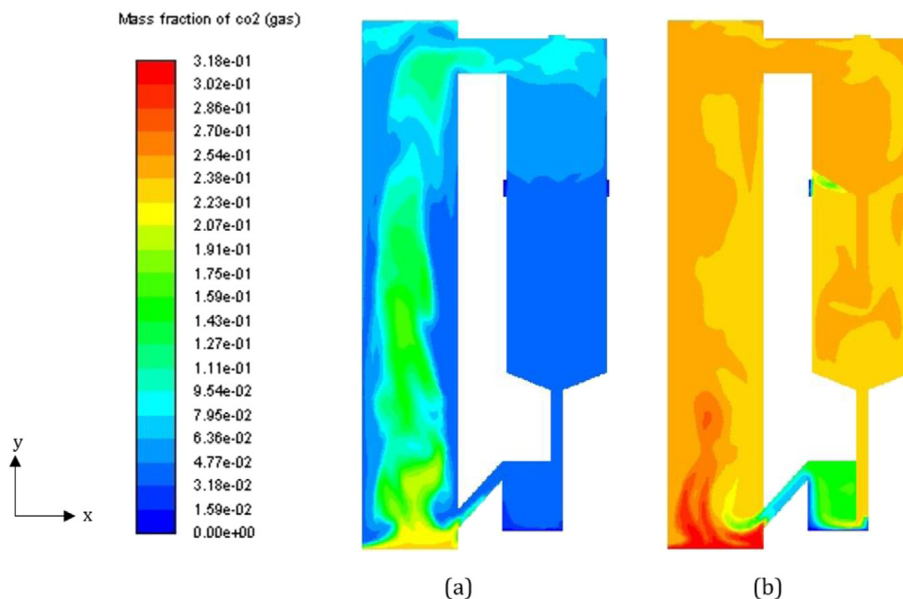


Fig. 7. Instantaneous plots of CO₂ mass fraction with different sources from (a) coal fired power plant and (b) cement industry.

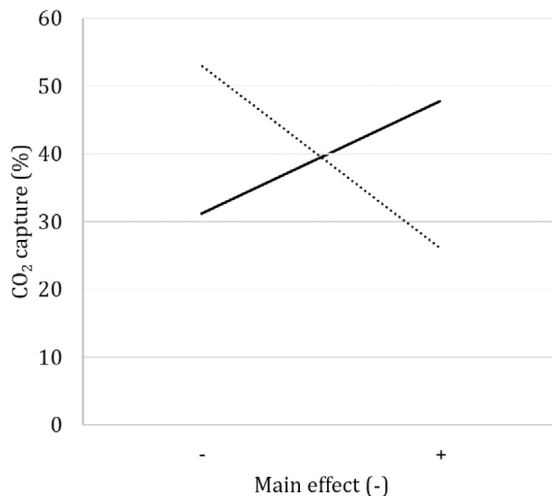


Fig. 8. Main effect plot of K_2CO_3 loading (straight line) at 0.128 and 0.5 and gas velocity (dotted line) at 1.5 m/s and 3.0 m/s on CO_2 removal efficiency.

4. Conclusions

A full loop of circulating fluidized bed reactor simulation was developed to obtain accurate system hydrodynamics. By comparison of the CO_2 removal efficiency, the results from simulation were agreed well with results from experiment. The results of hydrodynamics displayed that CO_2 was captured in adsorber and transformed to $KHCO_3$ while rich solid sorbents moved to regenerator for regeneration. Hydrodynamics in reactor was validated by compared with fluidization theory. Riser was operated in fast fluidized bed regime that particle mostly aggregated near the wall. In contrast, regenerator was operated in bubbling fluidized bed regime that solid volume fraction and velocity tended to constant. Different sources of CO_2 affected CO_2 removal efficiency. The CO_2 concentration for CO_2 capture process of flue gas from coal fired power plant was more captured than the cement industry with similar other conditions. The main effect plots showed that K_2CO_3 loading in solid sorbent had direct variation on the CO_2 removal efficiency while gas velocity had inverse variation.

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