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## Article

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# Dynamic model and control system of carbon dioxide capture process in fluidized bed using computational fluid dynamics

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## Abstract

Nowadays, the concentration of greenhouse gases in the atmosphere has been growing continuously due to the increase of energy consumption, generated from carbon-based fuels and has created global warming. In this study, a model of carbon dioxide capture adsorption in a fluidized bed reactor was developed based on experimental data using commercial CFD program called ANSYS FLUENT. Then the model was employed to observe the hydrodynamics behavior and the dynamic responses of CO<sub>2</sub> capture inside the adsorber when the operating variables were changed. The effects of operating variables on carbon dioxide capture were evaluated. From the simulation results, both the inlet gas velocity and the inlet solid circulation rate affected the carbon dioxide capture. The relationships between inlet gas velocity and inlet solid circulation rate to the percentage of carbon dioxide capture were investigated and analyzed by using system identification toolbox in MATLAB. After that, these relationships were used to design a control system. For the considered control system, the inlet solid circulation rate was selected to be a manipulated variable, while the inlet gas velocity, composition and temperature were designated as system disturbances. The controlled variable was carbon dioxide content remaining in the flue gas at the outlet. It was found that the control system could maintain the concentration of carbon dioxide in the flue gas at a specified value.

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*Keywords:* Carbon dioxide capture; Fluidized bed reactor; Solid sorbent; CFD; Adsorption; Control system

## 1. Introduction

Due to global warming, global temperature around the world will continue to rise. The main cause of the global warming is the releasing of greenhouse gases from industries, especially power plants, agriculture and others. These sectors use fossil fuels like coal, natural gas and oil in combustion processes. The majority of greenhouse gas

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emission in the United States is carbon dioxide (CO<sub>2</sub>) that accounted for about 81.6% from electricity, transportation and industries [1]. Consequently, the technologies for capturing CO<sub>2</sub> have been proposed worldwide. There are four main technologies for CO<sub>2</sub> capture produced from the power plants, which are pre-combustion, post-combustion, oxy-fuel combustion and chemical looping combustion. Post-combustion is the appropriate alternative because of its high performance and convenience compared to other technologies. Several efficient methods such as absorption, adsorption, membranes and cryogenic separation have been proposed to capture CO<sub>2</sub>. To date, many industries focused on capturing CO<sub>2</sub> by aqueous amines or monoethanolamine (MEA) solutions. Liquid amines provided high CO<sub>2</sub> capture capacities; however, they could be severely corrosive to equipment [2] and require large amount of energy for regeneration [3]. The amine solutions are expensive and are suitable for large-scale industries. On the contrary, the adsorption process that uses solid sorbent for CO<sub>2</sub> capture has many potential advantages such as cheap material and less energy required for regeneration. However, the adsorption capacity is lower than those of absorption. CO<sub>2</sub> in flue gas can be adsorbed on solid sorbents, like potassium carbonate (K<sub>2</sub>CO<sub>3</sub>) or sodium carbonate (Na<sub>2</sub>CO<sub>3</sub>), physically and chemically. In this study, Na<sub>2</sub>CO<sub>3</sub> was selected as adsorbent because it required low energy for regeneration [4].

A circulating fluidized bed reactor (CFBR) is commonly used as a chemical reactor for a multiphase flow system [5]. The CFBR had been developed to investigate the potential of CO<sub>2</sub> capture processes [6]. Since different hydrodynamics conditions inside the reactor provide different performance on the CO<sub>2</sub> capture, it was found that the circulating-turbulent fluidized bed (CTFB) regime could enhance the CO<sub>2</sub> capture [7]. Thus, the CTFB regime was investigated experimentally and numerically [8]. The CTFB regime took place under the condition between the conventional turbulent and fast fluidization regimes. The hydrodynamics of this regime has been researched in the previous literature [9]. The CTFB regime had a high mixing property and high CO<sub>2</sub> capture capacity for a real chemical reaction [10]. Numerical modeling is a powerful tool to investigate the hydrodynamics and performance of the adsorption process. Computational fluid dynamic (CFD) is a technique that uses numerical method to simulate the transport phenomena of multiphase flow systems. This method is attractive and feasible for performance analysis, design and optimization of multiphase reactors, especially, when the behavior of the system is complex and requires high cost laboratory experiment to perform. Due to the complication of the CFBR, in order to achieve the actual operating conditions of the reactor, the studies of its dynamic responses and that of how to control the reactor are inevitable and investigated. Dynamic responses and the control system of the CO<sub>2</sub> capture process involves with three variables including; the percentage of CO<sub>2</sub> in the outlet as a controlled variable, solid circulation rate as a manipulated variable, and the flow rate and composition of flue gas as disturbance variables. The controller will adjust the manipulated variable when the disturbance variables change [11]. Nevertheless, there are rare researches related to dynamics and control system of the CO<sub>2</sub> adsorption process under the CFD environment. As a result, this study aims to develop the dynamic model of CO<sub>2</sub> adsorption process that can imitate its actual behavior and to construct a control system that can compensate with the system deviations.

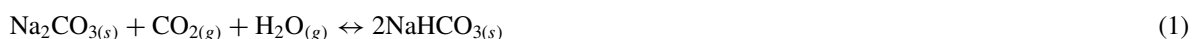
## 2. Mathematical model

### 2.1. Governing equations and constitutive equations

In this study, the circulating fluidized bed reactor was simulated based on a set of governing equations for conservation of mass, momentum, energy and species, and the constitutive equations was obtained from kinetic theory of granular flow theory as described by Thummakul et al. [10] and Boonprasop et al. [12]. The commercial CFD software, ANSYS FLUENT 19.1, was used to model and simulate the system.

### 2.2. Adsorption kinetic models

The solid sorbent, used in this study, was sodium carbonate which was occurred according to the equilibrium reaction as shown below in Eq. (1).



The sodium carbonate reacts with CO<sub>2</sub> and water vapor and forms the product, sodium bicarbonate (NaHCO<sub>3</sub>). In contrast, the CO<sub>2</sub> capture will be lower when the sodium bicarbonate reaches its decomposition pressure. At

this stage, the reverse reaction will occur. The rates of these reversible reactions are represented as the function of concentration of CO<sub>2</sub> and water vapor [12] as shown in Eqs. (2) and (3).

$$r_{fw} = k_{fw} [\text{CO}_2]^{0.4} [\text{H}_2\text{O}]^{0.4} \varepsilon_{\text{Na}_2\text{CO}_3}; k_{fw} = 1 * 10^{-10} \left[ e^{\frac{70}{RT}} \right] \quad (2)$$

$$r_{bw} = k_{bw} \left( \frac{1}{[\text{CO}_2]} \right)^{0.15} \left( \frac{1}{[\text{H}_2\text{O}]} \right)^{0.15} \varepsilon_{\text{NaHCO}_3}; k_{bw} = 7.83 * 10^{-3} \left[ e^{\frac{-0.000502}{RT}} \right] \quad (3)$$

### 2.3. System description and boundary conditions

A schematic drawing of the simulated two-dimensional adsorption reactor and the parameters used in the simulation are shown in Fig. 1 [10]. In this study, the 2D reactor geometry was generated by the DESIGN MODULER software. The dynamic simulation of multiphase flow was carried out with the Eulerian–Eulerian model. The governing equations were solved using the finite volume method, while the first order upwind schemes were applied to discretize all the governing equations. The phase coupled SIMPLE algorithm (Semi-Implicit Method for Pressure-Linked Equation) was utilized to solve the pressure–velocity coupling. The EMMS interphase exchange coefficient or drag model was employed to simulate the particle clustering phenomenon inside the system. The grid independence was also performed to determine the optimal grid number.

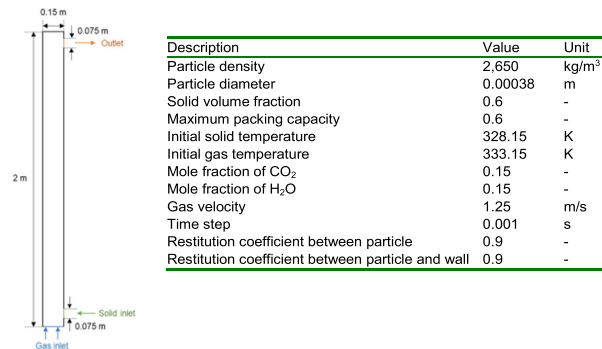


Fig. 1. Schematic drawing of the adsorption reactor used in this study and the operating conditions.

### 2.4. PID controller

The CO<sub>2</sub> adsorption control system was developed by using the system identification toolbox in MATLAB. The toolbox can generate transfer functions of process and disturbances from step response tests. The step response tests were introduced to the CFD model and the responses were supplied to the toolbox to obtain the transfer functions of the process and disturbances. After that, the process model, disturbance models and PID controller was employed using Simulink Toolbox in MATLAB software. The PID controller is the combination of three parameters including; proportional gain ( $K_p$ ), integral term ( $K_i$ ) and derivative term ( $K_d$ ). In this control system, CO<sub>2</sub> content at the outlet of the reactor was the controlled variable and the inlet solid circulation rate (in kg/m<sup>2</sup> s) to the reactor was the manipulated variable. The error signal ( $e(t)$ ) in Eq. (4) is operated in the non-interacting (parallel) form of PID controller that is shown in Eq. (5) [13]. In addition, the PID controller coefficients ( $K_p$ ,  $K_i$  and  $K_d$ ) were tuned for proper process responses before they were used for the control system.

$$e(t) = \text{desired output} - \text{current output} \quad (4)$$

$$\text{Controller output}(t) = K_p e(t) + K_i \int_0^t e(t) dt + K_d \frac{de(t)}{dt} \quad (5)$$

### 3. Results and discussion

#### 3.1. Mesh independency

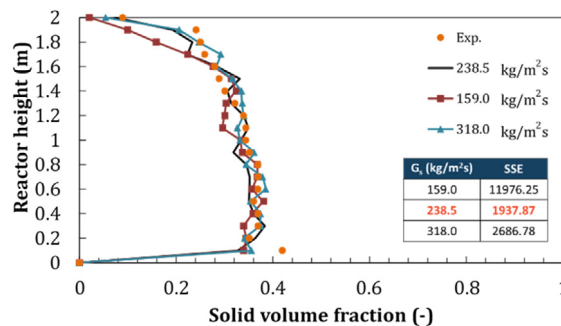
Table 1 shows the mesh independence test relating to the absolute pressure in the reactor. The mesh independence test was run at the inlet gas velocity of 1.25 m/s with varying mesh sizes; 3000, 6000, 9000 and 12,000. It was found from the obtained information that the optimum mesh size was 9000 meshes.

**Table 1.** Mesh independence at average time 20–40 s.

Mesh	Absoluter pressure at the middle of the reactor (Pa)
3,000	105,896.49
6,000	106,717.46
9,000	106,546.34
12,000	106,516.80

#### 3.2. Verification of the hydrodynamics model

To validate the model, the response of the cold model result was compared to the experimental data [9]. The solid circulation rate ( $G_s$ ) and inlet gas velocity ( $V_g$ ) (maintained at 1.25 m/s) values were referred from the real experiment. Fig. 2 shows the solid volume fraction profile along the reactor with different solid circulation rates. The predicted solid volume fraction profiles were compared to the experimental data. With these operating conditions, the solid volume fraction was homogeneously distributed and was slightly changed in the axial direction along the height of the reactor. The suitable solid circulation rate was 238.5 kg/m<sup>2</sup> s.



**Fig. 2.** Solid volume fraction profiles of the reactor in this study comparing with the experimental data quantitatively.

#### 3.3. Verification of the reaction model

The chemical reaction model of CO<sub>2</sub> adsorption had been validated with the previous literatures (Table 2). The validation indicated that the used reaction models were not suitable for this study. The main factor which caused the difference between the previous study and current simulation results was the size of the reactor. Thus, the tuning factor, the gain of the sorption, was required. The suitable tuning parameter value was 0.125 which gave the minimum errors compared to the literatures (Table 2).

**Table 2.** Verification of the reaction model.

Literature	CO <sub>2</sub> capture (%)	Tuning factor of kinetics model				
		0.080	0.100	0.125	0.150	1.000
Kongkitisupchai et al. [4]	68.00–82.00					
Boonprasop et al. [12]	67.32	55.16	63.64	68.32	72.32	98.90

**Table 3.** Effects of operating parameters on the percentage of CO<sub>2</sub> capture.

Run	V <sub>g</sub> (m/s)	G <sub>s</sub> (kg/m <sup>2</sup> s)	CO <sub>2</sub> capture (%)	Run	V <sub>g</sub> (m/s)	G <sub>s</sub> (kg/m <sup>2</sup> s)	CO <sub>2</sub> capture (%)
1	1.00	159.0	76.37	14	1.50	397.5	62.71
2	1.00	238.5	77.23	15	1.50	477.0	63.25
3	1.00	318.0	77.76	16	1.75	159.0	50.50
4	1.00	397.5	78.44	17	1.75	238.5	52.43
5	1.00	477.0	79.16	18	1.75	318.0	54.10
6	1.25	159.0	65.91	19	1.75	397.5	55.44
7	1.25	238.5	67.64	20	1.75	477.0	56.44
8	1.25	318.0	68.78	21	2.00	159.0	43.84
9	1.25	397.5	70.36	22	2.00	238.5	46.35
10	1.25	477.0	71.65	23	2.00	318.0	48.65
11	1.50	159.0	57.20	24	2.00	397.5	49.71
12	1.50	238.5	59.99	25	2.00	477.0	50.85
13	1.50	318.0	61.02				

### 3.4. Effects of operating parameters

This study determined the effect of operating parameters such as inlet gas velocity and solid circulation rate on the percentage of CO<sub>2</sub> capture. Concluded in Table 3, the percentage of CO<sub>2</sub> capture decreased when inlet gas velocity increased due to the decrease of the residence time of solid sorbent and the increase of the entering of CO<sub>2</sub> content in the reactor. On the other hand, the increase of solid circulation rate resulted in the increase of solid hold up and provided higher CO<sub>2</sub> adsorption capacity in the reactor. Referred to previous literature, the operating parameters that affected the CO<sub>2</sub> capture were the inlet gas velocity, the initial CO<sub>2</sub> content of inlet gas, the initial water vapor content of inlet gas, the inlet gas temperature and the solid circulation rate [10,14,15]. In addition, the CO<sub>2</sub> adsorption was exothermic reaction, thus when increased the inlet gas temperature, the performance for capturing CO<sub>2</sub> decreased [10]. On the other hand, when the water vapor of inlet gas increased, more CO<sub>2</sub> was removed because of the higher kinetic reaction rate [14]. The increasing solid circulation rate led to the increasing in the solid hold up that could adsorb more CO<sub>2</sub> in the reactor [15].

### 3.5. Simulation of step response test

In this study, the CTFB regime, with inlet gas velocity between 1.00 and 2.00 m/s, was considered [10]. Normally, the CO<sub>2</sub> content in the flue gas from fossil fuel utilization in a power plant was about 10%–20% [16]. In addition to CO<sub>2</sub> content, the moisture in flue gas was about 5%–16% [17,18]. The moisture of the flue gas in this study was then varied within 10%–20%. In addition, the adsorption temperature was also concerned in this study. The values were referred from the previous literatures [12,17] were in the range of 313.15–353.15 K. The last considered factor was the solid circulation rate which was defined in a range of 159–477 kg/m<sup>2</sup> s. The base case assumptions include; inlet gas velocity of 1.5 m/s, the initial CO<sub>2</sub> content of 15%, initial water vapor of 15%, the inlet gas temperature of 333.15 K and the solid circulation rate of 318 kg/m<sup>2</sup> s. The step response test was applied to evaluate the transfer functions of the process and disturbances (Fig. 3). The transfer function of the process was determined by applying step change of solid circulation rate (G<sub>p</sub>). With the same fashion, the transfer functions of disturbances were obtained by changing inlet gas velocity (G<sub>d1</sub>), initial CO<sub>2</sub> content (G<sub>d2</sub>), initial water vapor content (G<sub>d3</sub>) and temperature of inlet gas (G<sub>d4</sub>).

Fig. 3 shows process parameters and those of the PID controller, determined by auto tuning mode in MATLAB. These values, K<sub>p</sub>, K<sub>i</sub> and K<sub>d</sub> were –0.226, –0.218 and –0.019, respectively. The values of them were negative, it implied that the controller is in direct action mode.

### 3.6. Performance of dynamic and control system

From the PID controller tuning mentioned in the previous section, the values of K<sub>p</sub>, K<sub>i</sub> and K<sub>d</sub> can be used for the control system of the CO<sub>2</sub> capture process using ANSYS FLUENT by writing the user define format (UDF) code.

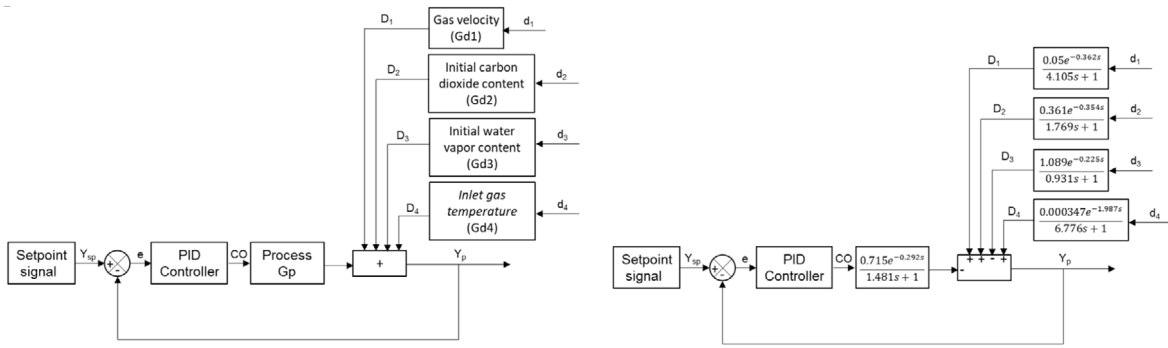


Fig. 3. The simulated model from step response test.

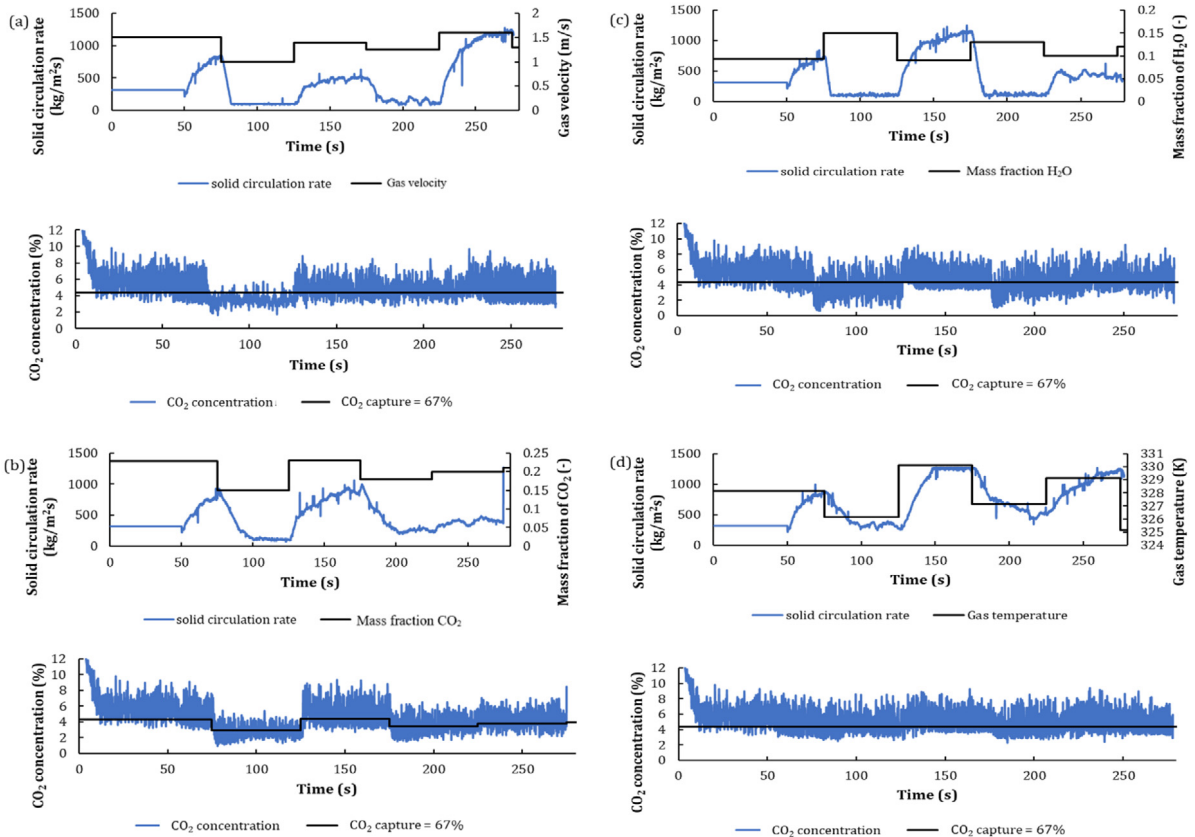


Fig. 4. Control performance when step of each disturbance variables and responsible of manipulated variable and controlled variable (a) gas velocity, (b) initial CO<sub>2</sub> content, (c) initial H<sub>2</sub>O content and (d) temperature.

In this study, the reactor was subject to disturbances of the gas velocity, compositions and temperature, which were assumed to take place by changing in combustion conditions of the power plant. Figs. 4 and 5 show the performance of the controller developed by writing UDF codes in ANSYS FLUENT when the disturbance changes. These cases assume that the percentage of CO<sub>2</sub> capture is 67 percent. For Fig. 4 shows the responses of the controller when gas velocity (Fig. 4a), initial CO<sub>2</sub> content (Fig. 4b), initial H<sub>2</sub>O content (Fig. 4c) and temperature (Fig. 4d) change, while Fig. 5 shows the responses of the controller when all of disturbances change.

In every case, disturbances were not introduced during the first 75 s. After 75 s, several disturbances took place every 50 s as shown until 280 s in Fig. 4 and 150 s in Fig. 5. The controlled variable could be maintained at the

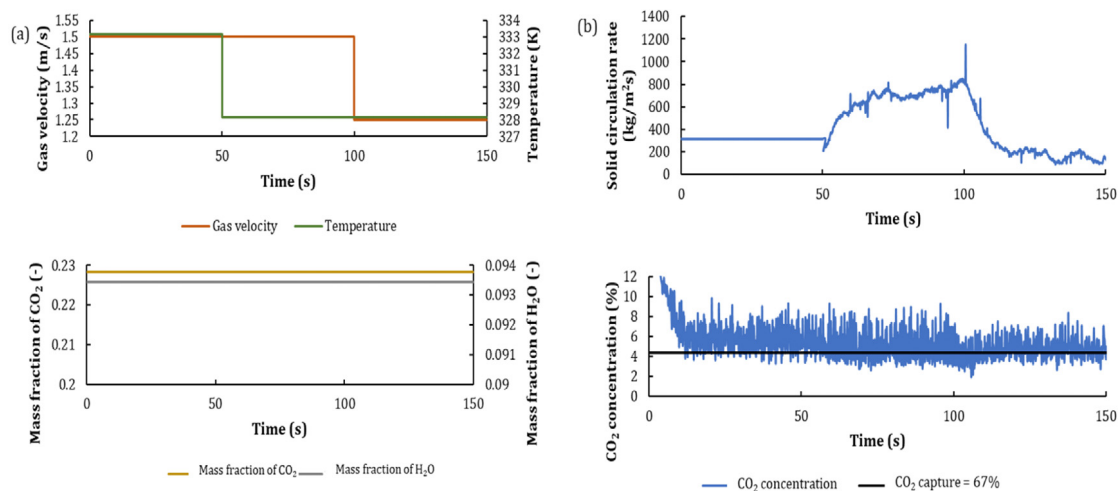


Fig. 5. Control performance (a) step of each disturbance variables and (b) responses of manipulated and controlled variables.

setpoint. As observed, the increasing in initial CO<sub>2</sub> content and inlet gas temperature or the decreasing in initial H<sub>2</sub>O content resulted in the increasing in solid circulation rate in order to maintain the CO<sub>2</sub> content at the outlet. On the other hand, when gas velocity decreased, solid circulation rate also decreased. Thus, the designed controller provided good responses when disturbances changed.

#### 4. Conclusion

Currently, there are few implementations of control systems for the CO<sub>2</sub> capture system with solid sorbent. In this study, the hydrodynamics and chemical reaction computational fluid dynamics models had been developed and validated by comparing the results with previous literatures. Then the model was used to develop transfer functions for control purposes. These transfer functions were employed to tune the controller for the CO<sub>2</sub> capture system. The tuned controller was tested its performances by applying changes of the disturbance for several conditions. It was found that the control system could move the system back to the set point after being disturbed.

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