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# Computational Fluid Dynamics Model of CO<sub>2</sub> Capture in Fluidized Bed Reactors: Operating Parameter Optimization

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## Abstract

Alternative energy is one of the methods for decreasing fossil fuel consumption. However, conventional fossil fuel process improvement is also considerably interesting issue due to the fact that adjusting existing process is easier and cheaper comparing to the development of the process compatible with the alternative energy. At present, the global warming and climate change phenomenon cause the increasing of average earth temperature. The CO<sub>2</sub> emission to the atmosphere is mainly produced by fossil fuel combustion from power industry. This is because the CO<sub>2</sub> has high heat capacity. Therefore, in order to use the conventional fossil fuel process efficiently, CO<sub>2</sub> should be eliminated from the flue gas before releasing it to the environment. Currently, there are many methods that use to capture CO<sub>2</sub> such as using circulating fluidized bed riser with solid sorbent. The advantages of circulating fluidized bed riser are uniform solid particle and temperature distributions, high contacting area between gas-solid particle and suitable for continuous operation. In this study, the effect of operating parameters on CO<sub>2</sub> capture in circulating fluidized bed riser with solid sorbent is investigated using 2D computational fluid dynamics model. The basic simulation step has to find the suitable computational mesh cells or grid independency test (5,000, 10,000, 15,000 and 20,000 cells) and compare the simulation result with the real experimental result. According to the simulation results, the suitable mesh cell is 10,000 cells and the obtained result is matched with the experimental results. Then, the effect of operating parameters on the CO<sub>2</sub> capture conversion is optimized.

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Keywords: Circulating fluidized bed reactor,  $CO_2$  capture; Computational fluid dynamics, Optimization;  $2^k$  factorial design.

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### Nomenclature

k

number of considered parameter

#### 1. Introduction

Nowadays, the emission of carbon dioxide (CO<sub>2</sub>) from chemical industry is a major cause of the global warming because CO<sub>2</sub> can absorb and maintain the heat which then has an impact on climate change. Currently, alternative energy is one of the methods for decreasing fossil fuel consumption such as solar energy and wind energy. It can decrease air pollution which is primary cause of the global warming, but the investment of equipment in building alternative energy plant is very expensive. Thus, conventional fossil fuel process improvement is also considerably interesting issue due to the fact that adjusting existing process is easier and cheaper comparing to the development of the process compatible with the alternative energy. There are many methods that use to capture CO<sub>2</sub> such as using circulating fluidized bed riser with alkali-based solid sorbent. Alkali metal carbonates such as Na<sub>2</sub>CO<sub>3</sub> and K<sub>2</sub>CO<sub>3</sub> react with CO<sub>2</sub> and H<sub>2</sub>O and transform to alkali metal hydrogen carbonates after CO<sub>2</sub> adsorption [1]. In fluidized bed reactor, the solid flow pattern is important quantitatively due to difference solid flow pattern will affect the rate heat and mass transfers.

There are many researches that study the effect of operating parameter on CO2 adsorption in circulating fluidized bed riser. Wang et al. [2] researched about CO<sub>2</sub> capture using potassium-based sorbents in circulating fluidized bed reactor at different inlet gas velocities using simulation method by considering effect of particle clusters. According to their results, the simulation with particle cluster effect predicted the system hydrodynamics similar to the experimental result more than the simulation without particle cluster effect. Yi et al. [3] studied the effect of operating parameters, gas inlet velocity, solid circulation rate and water content in feed gas, on CO2 removal percentage in circulating fluidized bed reactor by using K<sub>2</sub>CO<sub>3</sub> solid sorbent. As a result, the increase of the overall CO<sub>2</sub> removal is owing to the increasing solid circulation rate and water vapor content and the decreasing gas velocity. Zhao et al. [4] studied the effect of amount of K<sub>2</sub>CO<sub>3</sub> on CO<sub>2</sub> sorption capacity. The CO<sub>2</sub> sorption capacity increased when increasing the amount of K<sub>2</sub>CO<sub>3</sub>. Yafei et al. [5] investigated the CO<sub>2</sub> capture performance of some wood materials by using fluidized bed reactor. The component of employed wood materials was investigated by XRD which showed high  $K_2CO_3$  component. According the results, the  $CO_2$  capture capacity increased when the reaction temperature decreased (60 to 100°C) and mole ratio between water and CO<sub>2</sub> increased. Apart from the experimental method, the simulation method was used to study the CO<sub>2</sub> capture processes. Emadoddin et al. [6] simulated CO<sub>2</sub> sorption in circulating fluidized bed using deactivation kinetic model and compared the results with experimental information and other chemical reaction models. According the results, differential pressure from simulation result was similar to experimental result [3]. In addition, the deactivation kinetic reaction model predicted the CO<sub>2</sub> removal percentage accurately more than the other chemical reaction model. However, the systematically study of the effect of operating parameters on the CO<sub>2</sub> removal percentage is still lacking in the literature. Most of the studies were considered the experiment using one factor at a time methodology. With this methodology, the interaction effect between operating parameters cannot be obtained.

The main objective in this study is therefore to investigate the effect of the different inlet gas velocities and the solid circulation rate on the  $CO_2$  conversion using two-dimensional computational fluid dynamics model. The numerical model is comparing its correctness with the literature experimental data by Yi et al. [3]. In this study, the response surface via  $2^k$  factorial statistical experimental design (with literature base case condition) was found for determining the operating parameter optimization on the  $CO_2$  conversion in circulating fluidized bed reactor.

#### 2. Methodology

#### 2.1 Computational model

In this study, the circulating fluidized bed riser was constructed by using computer-aided design program, DESIGN MODULER and was simulated by using computational fluid dynamics simulation program, ANSYS FLUENT. The model in two-dimensional Cartesian coordinate system which consisting of 5,000, 10,000, 15,000, 20,000 mesh cells and 80 s flow time was used. The gas and solid particles entered to the circulating fluidized bed

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