Computational fluid dynamics simulation of novel flow regimes in high density circulating fluidized bed reactor

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Abstract – To maximize the carbon dioxide sorption efficiency in high density circulating fluidized bed reactor, the gas-solid particle flow regimes had been investigated using commercial computational fluid dynamics programs (GAMBIT and ANSYS FLUENT). The circulating fluidized bed reactor had the overall dimension of 2.00 m height, 0.30 m width and 0.05 m depth. The grid independency test was employed to study the effect of different grid or mesh size on the simulation result. The quasi-steady state operation of the system was detected from the result of grid independency test which was about 20 s to 40 s. The gas velocity was varied to investigate different flow regimes of the gas-solid particle. The results from the simulation showed that the solid particle volume fraction profiles were able to predict various flow regimes at each specific gas inlet velocity. The velocities of gas phase and solid phase were shown in this literature to provide the idea of the regime characteristic. The novel flow regime was appeared at gas inlet velocity from 0.75 m/s to 1 m/s. Due to its characteristic, this flow regime was the most appropriate regime for the carbon dioxide sorption application.

Keyword: Circulating fluidized bed reactor, Computational fluid dynamics, Flow regime

1. Introduction

Carbon dioxide is becoming a significant source of worldwide global warming problem due to their ability to maintain the heat inside the earth atmosphere. Recently, the fluidization technology has been used for reducing carbon dioxide from power generation and many other industrial processes. However, the complex hydrodynamics of the fluidization process is very difficult to understand. Not only its complication but also the cost for experiment with the real industrial scale is very expensive. The computational fluid dynamics (CFD) technique then plays an important role for solving this problem and has a potential to predict the phenomenon and flow characteristic inside the fluidized bed system. The computational fluid dynamics can be used in many kind of process from small to large scale equipment [1] and can be used in both 2D and 3D system. For the 2D system, the results are obtained faster while the 3D system can predict more accurate results. In the literature, the computational results inside the circulating fluidized bed reactor of dense bed were conducted [2-4]. Their results showed that the dense bed system was consisted of a dilute region, a transition region and a dense region. The bubbling bed, turbulent bed, fast fluidized bed, dilute bed, slugging bed and spouted bed are the conventional flow regimes in circulating fluidized bed reactor system [3-4]. In addition, there were many researches about the solid sorbent for carbon dioxide sorption using potassium carbonate. This is because potassium carbonate solid sorbent can easily regenerate with the temperature below 140°C [5] and can be economically and technically used when comparing to the other sorbents [6]. Kongporm and Gidaspow [7] studied the effect of different potassium carbonate feeding in circulating fluidized bed system. Their result showed that feeding the potassium carbonate uniformly at the flue gas inlet zone caused the disappearance of core-annular flow structure and increased the CO₂ capture efficiency. Comparing the potassium based sorbent with the other sorbents such as calcium based sorbent, by using calcium based sorbent for capturing carbon dioxide, the carbonation reaction had to be occurred in higher temperature system [8]. The experiments on the efficiency of the carbon dioxide absorption were also conducted in the literature. Zhao et al. [9,10] investigated the optimum condition for absorption and regeneration of carbon dioxide with potassium carbonate sorbent. From the absorption part, the proper temperature and pressure near the atmosphere condition gave higher conversion efficiency. Also, the concentration of the reactants had significant influenced on the absorption reaction. From the regeneration part, the increasing of heating rate greatly reduced the regeneration time and
conversion efficiency. However, most of the potassium carbonate researches were conducted in neither fixed bed reactor nor other reactors rather than fluidized bed reactor. This is why using the potassium carbonate in circulating fluidization reactor is become widely interesting for many research.

2. Research methodology

The considered computational system was conducted using GAMBIT software for creating the circulating fluidized bed reactor with the overall dimension of 2.00 m height, 0.30 m width and 0.05 m depth as shown in Fig. 1. In this system, the riser section had been used for taking place the carbonation reaction. The employed solid phase and gas phase properties are shown in Table 1.

Table 1. The employed solid phase and gas phase properties.

<table>
<thead>
<tr>
<th>Operating condition</th>
<th>Gas phase</th>
<th></th>
<th>Solid phase</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Gas velocity</td>
<td>0.50 - 4.00 m/s</td>
<td>Density</td>
<td>1.21 kg/m³</td>
</tr>
<tr>
<td></td>
<td>Viscosity</td>
<td>2.00 x 10⁻⁵ kg/m s</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solid phase</td>
<td>Density</td>
<td>2650.00 kg/m³</td>
<td>Viscosity</td>
<td>1.72 x 10⁻⁵ kg/m s</td>
</tr>
<tr>
<td></td>
<td>Diameter</td>
<td>210.00 microns</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Solid volume fraction</td>
<td>0.63 -</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Operating condition</td>
<td>Gravitational acceleration</td>
<td>9.81 m/s²</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The grid or mesh was investigated via the grid independency test with various grid or mesh sizes of 6,000 to 18,000. These reactors were imported to ANSYS FLUENT software for simulating and analyzing the phenomena inside the system. The potassium carbonate solid sorbent was used as a sorbent in this study. The Eulerian model was chosen to compute the mass and momentum conservation equations for each phase. The solid phase and gas phase inlet boundary conditions were defined as velocity inlet and the outlet boundary condition was defined as pressure outlet. The wall boundary condition was no slip for both phases. The energy conservation equation was excluded in the cold flow process which had the objective to determine the flow characteristic at different gas inlet velocities. The model had been set as transient model to detect the quasi-steady state condition in the reactor. The results were shown using the volume fraction and velocities at various heights to determine the flow regime at different gas inlet velocity.

Fig. 1. The overall dimension of circulating fluidized bed reactor.
3. Results and Discussion

The study on hydrodynamics in fluidization reactor had been conducted to investigate the flow behavior at different gas inlet velocities. The provided gas inlet velocities were 0.50, 0.75, 1.00, 2.00, 3.00 and 4.0, m/s to discover the novel regime for the carbon dioxide absorption system which requires continuous high density of sorbent. The preliminary results were conducted to define the effect of the gird or mesh. The quasi-steady state condition was found by analyzed the results from grid independency test as shown in Fig. 2 and 3.

Fig. 2 and 3 show the averaged solid volume fraction and pressure drop per unit length at different simulation times, respectively. The show results were example results at selected three gas inlet velocities. From the preliminary results, the variation of grid or mesh sizes after 6,000 cells did not change the observed results. Thus, the smallest one was selected to use in this study to minimizing the computation time. The quasi-steady state is determined by the point that the distribution of solid volume fraction and the pressure drop are stable. From the figures, the stable point was started at 20 s simulation time which means that the quasi-steady state was started after 20 s simulation time.

As stated above, ANSYS FLUENT software was used for simulation the high density reactor at various gas inlet velocities. In Fig. 4, the results are presented by the contours of solid particle volume fraction on the riser side which showed the solid particles behavior at several of gas inlet velocities at 40 s.

From each gas inlet velocity, the solid particles behavior seemed to have different characteristic. At the lowest gas inlet velocity, the solid particles were not yet re-circulated and there were many bubble of gas inside the system. At this moment, the bubbling fluidization was occurred at gas velocity of 0.50 m/s. From 0.50 m/s to 0.75 m/s, bed of potassium carbonate began to expand but still not re-circulated. The solid particles were moving disorderly in the flow regime called turbulent fluidization. From 0.75 m/s to 1 m/s, some of solid particles went into the cyclone section and separated down back into riser. Inside the reactor system, the solid particles almost had the same dense solid density distribution. This phenomenon was novel flow regime which was defined as circulating turbulent fluidization. With this flow regime, the solid particles were able to contact with the gas excellently. When the 1 m/s to 3 m/s of gas inlet velocities were supplied, the core-annular, some of the solid particles fell back especially at the wall and some of them flew upward at the center, occurred which...
was the characteristic of fast fluidization regime. In this study, the core-annular could be seen obviously at gas velocity of 3 m/s. Finally, the pneumatic transport fluidization was occurred from 4 m/s and so on of gas inlet velocity. This flow regime showed very dilute region all over the riser system. Fig. 5 shows the axial distributions of solid particle volume fraction with different gas inlet velocities. Similar to the contours, the results can be used for confirming the flow regime.

Fig. 4. Instantaneous contours of solid particle behaviour in riser with 0.50, 0.75, 1.00, 2.00, 3.00 and 4.00 m/s gas inlet velocities.

Fig. 5. Axial distributions of time-averaged solid particle volume fraction in riser with 0.50, 0.75, 1.00, 2.00, 3.00 and 4.00 m/s gas inlet velocities.
Fig. 6 illustrates the axial distribution of time-averaged solid particle velocity at 1 m height above the bottom of riser with difference gas inlet velocities. According to the results, the obtained solid particle velocity profile after 2 m/s showed significantly back mixing phenomena as can be seen by the difference of the solid particle velocity between the center and the near wall regions. The back mixing phenomena are occurring due to the solid particles in the center region are pushed upward by the high gas velocity. Consequently, some of the solid particles were fallen back at the side wall and re-mixed with the new feed solid particles. This phenomena is claimed as an unwanted phenomena for carbon dioxide capture process because it decreases the sorbent surface area and enhances the occurrence of solid particle cluster.

![Axial velocity profile of solid phase](image)

Fig. 6. Axial distributions of time-averaged solid particle velocity at 1 m height above the bottom of riser with difference gas inlet velocities.

![Instantaneous contours of gas velocity in riser](image)

Fig 7. Instantaneous contours of gas velocity in riser with 0.50, 0.75, 1.00, 2.00, 3.00 and 4.00 m/s gas inlet velocities.
Fig. 7 displays the instantaneous distributions of gas velocity in riser with different gas inlet velocities. At 0.50 m/s, the gas velocity was observed at the bottom and middle zones because the acting force of the gas was not enough to overcome the resistance force or pressure of the solid particle bed. As a result, the gas caused the solid particle bed to move disorderly and the bubbling fluidization regime was occurred. At 0.75 m/s gas inlet velocity, the gas velocity started to gather at the center of riser. As stated above, the flow distribution with this gas inlet velocity was circulating turbulent fluidization regime. At 1.00 to 3.00 m/s which the fast fluidization regime was occurred, the gas velocity was gathered at the center of the riser which verified the occurrence of core-annular flow structure. The gas velocity was expanded with the increasing of gas velocity due to the reduction of solid particles. At 4.00 m/s of gas inlet velocity, the gas velocity all over riser increased and distributed all the entire riser. This can be explained by the decreasing of concentration of solid particles and the increasing of space for gas phase.

Fig. 8. Instantaneous contours of solid particle velocity in riser with 0.50, 0.75, 1.00, 2.00, 3.00 and 4.00 m/s gas inlet velocities.

Fig. 8 shows the instantaneous distributions of solid particle velocity in riser with different gas inlet velocities. The solid particle velocity distributions were consistent with the providing gas velocity. At 0.50 m/s of gas inlet velocity, the solid particles were rapidly moving at the bottom while slowly moving at the top. This is due to the distance from the enter zone. With this gas inlet velocity, some of the gas was able to penetrate through the solid particle bed as a bubble which is the characteristic of bubbling fluidization regime. At 0.75 m/s, the solid particle bed was risen up to the exit zone and moved disorderly. The solid velocity in the riser was almost the same in this novel flow regime. At 1.00 m/s, the solid particles were able to reach the exit zone and some of them were return to the bottom of the riser. As the gas inlet velocity increased from 1.00 to 3.00 m/s, the gas with high velocity could penetrate through the solid particle bed and even took some particle with it. At 4.00 m/s, the void zone of the solid particle phase had been detected because of the reduction of solid concentration. As stated above, the gas velocity larger than 4.00 m/s as providing in this study leading to pneumatic transport.

From the result, the most appropriate regime for the carbon dioxide sorption system is circulating turbulent fluidized bed which is occurred from 0.75 m/s to 1 m/s. This regime does not only appropriate for carbon dioxide sorption system but also suitable for other systems which require high multiphase contacting surface area for example drying process.
4. Conclusions

In this study, the new flow regime of high density circulating fluidized bed reactor were observed using computational fluid dynamics simulation called the circulating turbulent fluidized bed. This flow regime is suitable for the carbon dioxide sorption and other applications which require high multiphase contacting surface area. With this flow regime, there had high and continuous volume fraction of potassium carbonate all over the riser. However, there are still many parameters effecting on carbon dioxide sorption. Therefore, more extension studies are needed to support the result in this study.

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