EFFECT OF PRESSURE ON FLOW BEHAVIORS IN DENSE GAS-FLUIDIZED BEDS: A DISCRETE PARTICLE SIMULATION STUDY

Jie Li and J. A. M. Kuipers

Fundamental Aspects of Chemical Reaction Engineering
Department of Chem. Eng. Twente Univ. of Tech,
7500 AE, Enschede, The Netherlands

ABSTRACT
A computational study has been carried out to assess the influence of pressure on the flow behaviors in dense gas-fluidized beds. Therefore the discrete particle simulation approach has been employed to study the regime transitions, local two-phase flow structures and the energy dissipation distribution. The results show that high pressure reduces the incipient fluidization velocity, widens the uniform fluidization regime and leads to a quick transition to the turbulent regime. Particularly it is discovered that high pressure, through enhancing gas-solid interaction and reducing the particle collision frequency, efficiently suppresses formation of large bubbles. As a consequence thereof more uniform gas-solid flow structures are produced leading to particulate fluidization.

INTRODUCTION
Many of the industrial fluidized bed units are operated at elevated pressure. The effect of pressure on two-phase flow behavior is of significant practical interest. Although many studies have been conducted, the detailed gas-solid flow behavior in gas-fluidized beds at elevated pressure is still unclear due to the experimental difficulties. Yates (1) and Knowlton (2) have given reviews on the pressure influences in gas-fluidized beds. Very recently, by employing X-ray techniques, Gilbertson et al. (3, 4) discovered that many aspects of the bubble behavior at high pressure, such as the bubble formation, the development and the eruption as well as its internal structures, are quite different from those at atmospheric conditions. Due to advances in computer hardware and simulation techniques, now it is possible to carry out the two-phase flows dynamic simulation on a single particle resolution. The role of particle-particle interaction and particle-fluid interaction and thus of internal mechanisms controlling the flow structures and regime transitions can now be studied theoretically in great detail.

At present stage, there are two main discrete particle simulation approaches available: one is the Discrete Particle Simulation (DPS)/molecular dynamics simulation approach or the so-called “hard-sphere model”, which has been developed by Hoomans et al. (5). This model is very suited to describe the suspended particle system, such as gas-fluidized beds. In this model, the particle collisions are treated as binary, instantaneous, inelastic collisions with friction. The other one the so-called “soft-sphere model” or
Discrete Element Method (DEM) treats the particle collisions as multiple, endurable, inelastic collisions with friction. It is suited especially to describe granular flows as encountered in mixers and hoppers.

This research aims at understanding the effect of pressure on the gas-solid flow behavior in gas-fluidized beds by employing discrete particle simulation techniques. Firstly, two parallel sets of simulations, one at atmosphere condition and one at elevated pressure condition, were carried out to elucidate the effect of pressure on regime transitions by comparing bed pressure drop. In addition, the pressure influences on gas bubble behavior in the same flow regime were examined to understand how the pressure influences the local flow structures and produces a uniform two-phase flow. Furthermore, the amount of energy, dissipated in the processes of the particle-particle and particle-wall collisions and the particle-fluid friction were determined to gain insight how pressure affects gas-solid-solid interactions at the different system pressures. Accordingly, we might understand 1) the role underlying macro-scale flow patterns and flow regime transitions and 2) the pressure effect on the level of particle.

THEORETICAL BACKGROUND

Governing Equations
In our discrete particle simulation the gas phase is treated as a continuous phase and described by the volume averaged Navier-Stokes equations whereas the particles are described on the basis of their Newtonian equations of motion. The governing equations are the same as those employed by Hoomans (6). The original codes for solving these sets of equations were developed by Kuipers (7) for gas flow and Hoomans (8) for granular dynamics, including both 2D and 3D. Additionally, the code for granular temperature calculation was developed and supplemented in this research.

Simulation Technique
The collision model originally developed by Wang and Mason (9) and later on improved by Hoomans et al. (3), is used to describe a binary, instantaneous, inelastic collision with friction. The key parameters of the model are 1) the coefficient of restitution (0 < e < 1) and 2) the coefficient of friction (μ > 0). The bed pressure drop is obtained by calculating the pressure difference between the bottom and top portion of the bed. Because of the pressure drop fluctuations, especially in the bubbling fluidization regime, statistical treatment of the data was required to obtain the time-averaged pressure drop. The standard deviation of pressure signal, defined in equation 1, was used as a parameter for determining the flow regime transitions. Where T and P represent time and pressure respectively.

\[ s = \sqrt{\frac{1}{T} \sum_{i} (p_i - \bar{p})^2} \]  

The simulation conditions are listed in Table 1.

RESULTS AND DISCUSSION

Effect on Flow Patterns (structures)

High pressure may change particle-particle and particle-fluid interactions, which would lead to the different flow patterns. These patterns, or alternatively heterogeneous
structures, have a pronounced effect on gas-solid contacting. As a first step, the following simulations at the same flow regime but different pressure were carried out to understand this effect: 1) immediately above incipient fluidization point (homogeneous fluidization regime), 2) bubbling regimes and 3) near turbulent regimes.

Immediately above the incipient fluidization point there exists a homogeneous flow structure in the high-pressure case (21 bar) whereas on the contrary no homogeneous gas-solid patterns are found at atmospheric conditions (1 bar). In the latter case, occasional small bubbles or voids passed through the bed with a relatively lower bed height compared to the high pressure case.

Figures 1a and 1b show the simulation results obtained in the bubbling regime at 1 bar and 21 bar respectively. The heterogeneous gas-solid two-phase flow structures at atmosphere conditions, characterized by the presence of big bubbles, dominate the two-phase flows. On the contrary, at the high pressure case the voids are best described as swirling tongue-shaped masses containing gas and solids with no stable boundary which corresponds to the experimental findings of Fan and Danko (10). Thus, the higher pressure efficiently depresses the bubble growth and as a consequence thereof produces a more uniform gas-solid flow structure. Meanwhile, the bed height for the high pressure case is higher too, indicating more free space for each individual particle. Figures 2a and 2b show the simulation results near the turbulent regimes at 1 bar and 21 bar respectively. Once again the flow patterns for the high-pressure case display the uniform two-phase flow structures. Interestingly, bed pressure drop is characterized by lower amplitude but higher frequency, indicating that there still exist heterogeneous local flow structures. However, they are much smaller compared to those obtained in the low pressure case and in the range of meso-scale size. Additionally the simulation shows that the particle-particle collision frequency for the high-pressure case is much less compared to the corresponding low-pressure case. This evidence once again elucidates that fewer particle-particle encounters prevail at elevated pressure.

**Effect on the Regime Transitions**

Simulations at the various flow regimes were carried out by employing the hard-sphere model and the results of the variation of the bed pressure drop with superficial velocity are shown in Figures 3a and 3b at 1 bar and 21 bar respectively. It should be stressed here that the gas phase turbulence was not taken into account in this simulation.

By comparing the flow regimes obtained at high pressure and atmospheric conditions, we can draw the following conclusions. 1) The standard deviation of the pressure drop signal at elevated pressure is higher than that for the atmospheric case demonstrating that elevated pressure produces a more homogeneous two-phase flow. 2) High pressure reduces the incipient fluidization velocity, at our simulation conditions from 0.3 m/s at 1 bar to 0.105 m/s at 21 bar. The incipient fluidization point in the elevated pressure case could be predicted satisfactorily. 3) There exists a wider homogeneous particulate-fluidization regime (0.105-0.25 m/s at 21 bar and 0.30-0.40 m/s (pseudo-homogeneous) at 1 bar) but more narrow bubbling regime in the high pressure case compared to atmospheric conditions. 4) At elevated pressure increasing gas velocity more easily leads to the transition of the fluidization regime from bubbling to turbulent (0.9 m/s) indicating that high pressure shortens the bubbling regime, 5) The simulated pressure-drop values agree well with the theoretically predicted pressure drops. The deviations near the incipient fluidization point are owing to the contribution of gas phase and the
friction loss between fluid and the bed wall, which is relatively remarkable at the high pressure case.

Effect on Fluid-Particle-Particle Interactions

The results mentioned above demonstrate that elevated pressure significantly affects the hydrodynamics of the gas-solid two-phase flows both from the macro-scale and from the meso-scale point of view and tends to form the particulate fluidization. Then, why and how does it introduce such a remarkable change? As we know, there are three kinds of interactions in dense gas-particle flows: 1) and 2) internal interactions in both the solid phase and the gas phase and 3) particle-fluid interactions. Therefore, detailed examination of these interactions from a micro-scale point of view at the different operation conditions would help us to understand the influencing mechanisms. For the gas-solid two-phase flow operating at low gas velocity, it is important to consider 1) particle-particle interactions and 2) particle–fluid interactions which will subsequently be examined in more detail.

EFFECT ON THE PARTICLE-PARTICLE INTERACTION

By employing the granular temperature, defined similarly as in kinetic theory of granular flow, we obtained the interaction distribution in the gas-fluidized beds. Figure 4 presents two snapshots of the granular temperature distribution in gas-fluidized beds corresponding to flow structures prevailing at 1 bar and 21 bar respectively. From the figures we can clearly see that elevated pressure produces a very uniform distribution with lower value, i.e. moderately intense particle-particle collisions. On the contrary at atmospheric pressure a pronounced non-homogeneous distribution is obtained indicating intense interactions between the particles. Particularly, the most intensive particle collisions prevail in the regions around the bubbles where the granular temperature can be eight times higher than that of the surrounding emulsion phase. Additional statistical analysis revealed that that the time-averaged granular temperature possesses a wider frequency distribution at 1 bar than at 21 bar, suggesting that larger bubbles are responsible for these intense particle-particle collisions. Detailed information about the particle-particle interaction in gas-fluidized beds, including bubble, jet, pressure induced interactions, will be reported in another paper (Li and Kuipers, 11).

EFFECT ON PARTICLE-FLUID INTERACTION AND ENERGY DISTRIBUTION

Since the particle-fluid interaction accounted for in our model is based on a semi-empirical formula as used by Hoomans (5), it is impossible at this stage to directly obtain insight on this issue from the simulation. However, by comparing the two kinds of energy dissipated due to particle-particle interaction and fluid-particle interaction we can understand indirectly this interaction from the macro-scale because both sources of energy dissipation can be easily obtained from molecular dynamics based discrete particle modeling. Additionally, the pressure influences on the gas-solid two-phase flows can be elucidated.

Figure 5 presents the results of the energy analysis obtained at pressures of 1 bar and 21 bar. Here $f$ represents the ratio of one kind of particle energy to the particle total energy, drawing from gas phase by drag force and the initial particle energy. Three main kinds of energy distributions are displayed in Figure 5, including kinetic, potential, dissipation energy due to particle collisions (i.e. slide and stick between the particles). Apparently, there are very remarkable differences for the energy distribution for particle collision dissipation and suspension at two system pressures. The suspension energy at
21 bar is up to 90% of the total energy input in 10 seconds, against 40% for the corresponding value at 1 bar. Meanwhile, at the high-pressure case most of energy was distributed on increasing the particle potential energy, i.e. increasing bed height. Additionally, the particle kinetic energy is increased even though not so remarkable. This finding demonstrates that the higher pressure enhances the gas-solid interaction and suppresses the particle interactions. Since more energy is spent on particle suspension at elevated pressure it results in higher bed heights. Detailed energy dissipation analyses in gas-fluidized beds will be presented in a forthcoming paper (Li and Kuipers, 12).

Although the high pressure does not directly change the particle-particle interaction (due to the rigidity of the particles), through increasing gas density, the gas-particle interaction (drag force) increases. This intensification promotes the particles to obtain more energy to suspend themselves in the gas flow and to provide themselves more movement space, which consequently efficiently reduces the chance for particle-particle collision. The larger the particle the more pronounced this effect becomes. Meanwhile, a denser gas depresses the originally freely moving particles (larger drag force) which furthermore leads to less particle collisions. By this way, the high pressure successfully changes the role of the particle-particle inelastic collision and particle-fluid interaction in their competition process. As a result, it leads to a relative homogeneous flow field. However, owing to the existence of non-ideal collisions small bubbles still appear but they are much smaller than those in the atmospheric case. It is also discovered from the simulated particle layout that the solid mixing in the high pressure case is not so intensive compared to the atmospheric case which is due to the different bubble behaviors.

Based on the above understanding, it is inferred that the normal fluidized beds are very suitable to solid phase processes, such as particle mixing. On the other hands, fluidized beds operated at elevated pressure would offer advantages for systems requiring good gas-solid contacting, such as FCC regeneration.

CONCLUSION
By employing the discrete particle method, the effect of pressure on gas-solid two-phase flow behaviors with respect to flow patterns, regime transitions, and particle/particle/fluid interactions was examined. The following conclusions can be drawn: 1) Elevated pressure results in a homogeneous flow pattern in near incipient fluidization regime, smaller bubbles in the bubbling regime and a relatively homogeneous structure near the turbulent regime; 2) High pressure moves the incipient fluidization point ahead, extends the uniform fluidization regimes, and shortens the bubbling regime; 3) In comparable flow regimes, elevated pressure, through increasing gas density, intensifies the particle-fluid interaction, suppresses the particle-particle interactions and therefore raises the bed height. As a result, it promotes the gas-solid system to form a more homogeneous two-phase flow structure.

ACKNOWLEDGEMENT
The authors would like to acknowledge Dutch National Science Foundation for financial support and Dr. B. P. B., Hoomans for many times of helpful discussions.
REFERENCES


8) Hoomans, B. P. B., 2000, Granular dynamics of gas-solid two-phase flows, Ph. D dissertation, Twente University, Enschede, Netherlands.


Table 1. Simulation conditions for pressure influence on gas-solid flow in gas-fluidized beds

<table>
<thead>
<tr>
<th>Bed geometry:</th>
<th>Width (cm) × Height (cm)</th>
<th>10 × 40 ~ 80</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particles:</td>
<td>Diameter (mm), Density (kg/m³)</td>
<td>0.949, 1170</td>
</tr>
<tr>
<td></td>
<td>Number [-]</td>
<td>16,000</td>
</tr>
<tr>
<td></td>
<td>Incipient fluid. vel.(m/s)</td>
<td>0.301 (for 1 bar), 0.105 (for 21 bar)</td>
</tr>
<tr>
<td>Simulation:</td>
<td>Grid</td>
<td>20 × 40 or 80 cells</td>
</tr>
<tr>
<td></td>
<td>Total time (s) &amp; Time step (s)</td>
<td>10, 1×10⁻⁴</td>
</tr>
<tr>
<td></td>
<td>Restitution Coef.: Norm. (p-w &amp; p-p)</td>
<td>0.95 or 0.00 (ideal)</td>
</tr>
<tr>
<td></td>
<td>Friction Coef.: Norm. (p-w &amp; p-p)</td>
<td>0.30 or 0.00 (ideal)</td>
</tr>
<tr>
<td></td>
<td>Friction Coef.: Norm. (p-w &amp; p-p)</td>
<td>0</td>
</tr>
<tr>
<td>Operation conditions</td>
<td>Superficial gas vel. (m/s)</td>
<td>For 1 bar: 0.05 ~ 3.0</td>
</tr>
<tr>
<td></td>
<td>Static bed height (m)</td>
<td>0.15</td>
</tr>
<tr>
<td></td>
<td>Porosity at incipient fluidization [-]</td>
<td>0.4</td>
</tr>
<tr>
<td></td>
<td>Pressure (bar)</td>
<td>1, 21</td>
</tr>
</tbody>
</table>
Fig. 1: Typical flow structures computed in the bubbling regime: pressure effect
a) 1 bar, 2.7\(U_{mf}\); b) 21 bar, 3\(U_{mf}\)

Fig 2: Flow structures near turbulent regime at
(a) 1 bar, 8\(U_{mf}\) and (b) 21 bar, 8\(U_{mf}\)

Fig 5: Energy analysis in gas-fluidized beds: pressure influence

\[ E_{tot} = E_{sp} + E_{pot} + E_{kin} + E_{rot} \]

\( f_{i,j} \) = \([ E_{i,j} / (E_{tot} + E_{r, j}) ] \)
Fig 3: Simulated flow regimes at different pressures
a) atmospheric, 1 bar;  b) elevated, 21 bar

Fig 4: Granular temperature distribution in fluidized beds operating at
(a) 1 bar, 3U_{mf};  (b) 21 bar, 2.7 U_{mf}
KEY WORDS

Gas-fluidized bed, Elevated pressure, Discrete particle simulation, Flow structure, Regime transition, Energy analysis