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Numerical simulation of Lithium-Titanium gas-solid fluidized beds with MFIX and assessing the effects of pressure, particle size and inlet gas velocity on its performance

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ABSTRACT

Gas-solid fluidized beds (GSFB) have been investigated by many researchers due its high importance in the industry. Many efforts, both experimentally and theoretically, have been made to predict their behavior. Due to differences in the particle sizes, particle segregation is a common phenomenon in the gas-solid fluidized beds. Particle segregation affects the efficiency of heat transfer and mass transfer in the fluidized bed. In order to prevent the hot-spots and degradation of products in the fluidized bed reactors in which exothermic reaction occurs, proper mixing in the bed is required. To improve the efficiency of these processes at high pressures, in depth understanding of segregation and mixing phenomena are required. Therefore, it is the aim of this work to examine the effect pressure, particle size and gas inlet velocity on mixing and segregation parameters in these beds. To obtain these objectives, a commercial computational fluid dynamics package namely MFIX were utilized and Paraview was also employed to analyze the data. The findings of the present study reveal that computational fluid dynamics is a powerful tool for assessing the parameters affecting the performance of fluidized beds.

KEYWORDS

GSFB;
Particle segregation;
CFD;
MFIX;
Paraview.

INTRODUCTION

The hydrodynamics of gas-solid fluidized beds fluids are very complex in nature as the result of gravitational force between individual particles and the force between the particle and gas. As a result, adequate testing and producing rich data on the particle scale are not feasible. Upward motion of bubbles through the fluidized solid bed leads to mixing and segregation of bed particles. When bubbles go up through the bed, solid particles are drawn into the stationary part of the bubble wake. When particles from the bubble wake fall into the bed and new particles from the dense area around are drawn into the sequence, axial mixing occurs. When the bubbles reach the surface of the bed they get collapsed and the particles along the wake fall down onto the surface. Through such a mechanism, particle on the bed are mixed with particles above the bed. When bubbles go up in the bed they create empty spaces that are filled by particles falling from around bubbles. Mixing and segregation are immediate phenomena and are the result of balance in the bed, concentration gradient in the axial direction and uniform particle distribution in the radial direction[1]. In beds where there is size distribution, particle segregation is the result of difference in drag force per unit particle mass[2]. Several models have so far been presented to adequately describe mixing and segregation in beds. Some of these models address jetsam and flotsam particle concentrations in stable conditions. Model presented by Gibilaro and Rowe[1] is the starting point in forecasting concentration profiles in fluid beds with bubbles[3-8]. In this model, bed particles are distributed between two phases: bulk phase, which includes most of the solids and the wake phase that contains solids trailing the gas bubbles rising through the bed. Furthermore, in this model the particles are assumed to be only of two types of flotsam and jetsam. For the mass balance, particle transport mechanisms including circulation, exchange, axial mixing and segregation are considered. In the gas-solid fluidized beds, circulation is the movement of solid particles from the bottom to the surface of the bed by the wake phase. Therefore, the movement of solids between the bulk and wake phase is proportional to the concentration difference between the two phases where axial mixing is defined as a pseudo-diffusion mechanism. As demonstrated by Naimer and co-workers this term could be omitted from the mass balance, since it does not include any physically realistic mechanism in a fluidized bed[3]. To improve the efficiency of these processes at high pressures, in depth understanding of segregation and mixing phenomena are required. Therefore, it is the aim of this work to examine the effect pressure, particle size and gas inlet velocity on mixing and segregation parameters in gas-solid fluidized beds using MFIX software.

PRESSURE EFFECT

Fluidized beds that operate at high pressures have several advantages such as high rates of heat transfer, low particle segregation and small equipment size[9-10]. High pressure leads to an increase in the gas density which affects the forces between particles and fluid and the flow patterns. Therefore, the efficiency of gas-solid beds at high pressures is different from the normal conditions.

Research on gas-solid fluidized beds operating at high pressures has begun from 1970 and they demonstrated that dense beds exhibit smoother fluidization with tiny bubbles[11-13]. Researchers have demonstrated that an increase in the pressure enhances the rising velocity, frequency, the average volume fraction of bubbles and the rate of contact accordingly; however, it reduces the size of the bubbles[14,15]. Hoffman and co-workers from the cross section of the fluidized bed have shown that the bubble flow is centered in the axial direction of the column[16].

Some reserchers has been observed that the bubble break occurs more at higher pressures and in the lower part of the bubble[17,18]. It has also been reported that in gas-solid fluidized beds at high pressures, the beds are more extended and the particulate regime occurs in a larger zones[26-11]. The effect of pressure on system parameters other than the minimum fluidization velocity and in beds of smaller particles (i.e., group A), is higher than in beds of larger particles (groups B and D)[12,13].

For particles in gas-solid fluidized beds in group B, the assessment of pressure on gas bubble behavior is more complicated. An increase of pressure up to 16 bars would increases the bubble size accordingly[15,16,24,25]; however, further increase in the pressure decreases bubble size. They also repoted that x-ray photography could reveal the hydrodynamic aspects of bed bubbles (i.e., the bubbles formation, structure formation, growth and break-up).

MECHANISMS OF SEGREGATION

In this work, three different mechanisms have been found to be efficient in expressing relative motion of particles in the gas-solid fluidized beds. Rising of particles in the wake of a rising bubble not only is a mixing mechanism for particles, but also it is the main mechanism of particle segregation. However, only flotsam particles could be transferred to the upper part of the bed and for larger and heavier particles of jetsam. Downward movement of particles occurs through two mechanisms; either particle comes down by falling within the bubbles or penetrating the layers between particles. It is worth noting that the main cause of separation is the difference between the magnitudes of drag per unit weight of different particles. Thus, particles having higher drag per unit weight move to the bed surface while particles with lower values move toward the distributor.

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Parameters influencing segregation

Many features affect the complex phenomenon of segregation in gas-solid fluidized beds including: pressure, inter-particle density ratio, size ratio, particle shape, the minimum fluidization velocity, distribution of fluidization gas, the bed height to diameter ratio. WU and co-workers concluded that when the ratio of bed length to diameter was low, segregation increases[32]. Furthermore, an increase in the particle size, density or reductuin in the operating pressure, would enhances the segregation of particles accordingly[32]. In this work and amongst the above parameters, the effect of particle size and gas inlet velocity was investigated.

Segregation index

Rowe and co-workers defined the mixing index for a binary system as $M = \frac{(X_J)_u}{\overline{X_J}}$[33], where $(\mathbf{X_J})_\mathbf{u}$ is the fraction of jetsam particles in the upper part of the bed and $\overline{X_J}$ is the fraction of jetsam at the state of perfect mixing. Both and are expressed as weight fractions. However, when complete mixing or segregation occurs in the bed, the mixing index is either 1 or 0, respectively.

In 1982, Chiba and co-workers defined segregation index for a binary system as follows[34]:

$$S = \frac{(X_f)_u}{\overline{X_f}} \tag{1}$$

where is the flotsam weight fraction of particles in the upper part of the bed and is the flotsam weight fraction at the state of perfect mixing. In addition, when S is either 1 or 0 it means complete segregation or mixing, respectively. Coorelation exists between the above parameters and are defined as:

$$\overline{X_f} = 1 - \overline{X_J} \rightarrow M = \frac{1 - S\overline{X_f}}{1 - \overline{X_f}} = S + \frac{1 - S}{\overline{X_J}} \tag{2}$$

Evaluation of segregation in fluidized beds

Particle segregation in gas-solid fluidized beds has been studied by Goldschmidt in a binary bed and the following correlation has been proposed[35]:

$$s = \frac{S - 1}{S_{max} - 1} = \frac{\frac{h_{small}}{h_{large}} - 1}{\frac{2 - x_{small}}{1 - x_{small}} - 1} \tag{3}$$

where, and are the average height reached by small and large particles in the bed, respectively and are defined follows:

$$h_{small(large)} = \frac{\sum_{i=1}^{M} h_i ep_{small(large)_i}}{\sum_{i=1}^{M} ep_{small(large)_i}}$$

$$\begin{cases} M = total\ cells\ of\ bed \\ i = number\ of\ cell \end{cases} \tag{4}$$

For the bed under investigation in this work, since the same volume percentage of the two particles with the same density was present in the bed. Furthermore, the pattern of segregation in the bed was also examined under different operating conditions.

For smaller particles of identical densities, the average mass fraction was evaluated from the following relationship:

$$x_{samall} = \frac{ep_{small}}{ep_{small} + ep_{large}} \tag{5}$$

Numerical methods

MFIX software

MFIX is a commercial computational fluid dynamics package whose general goal is to describe the hydrodynamic simulation of chemical reactions and heat transfer in gas-solid, dense or dilute flows usually occurring in the energy conversion and chemical processing reactors[17]. MFIX was developed by the US National Energy Technology Laboratory in FORTRAN and could model systems of multiple particle types, two or three dimensional Cartesian or cylindrical coordinate systems, and systems involving heat transfer and mass transfer. MFIX presents information on pressure, temperature, composition, and velocity distributions of systems as a function of time. In 1996, MFIX code was used in studies in order to enhance the accuracy of calculations, execution speed and simulation of fluidized bubble bed. In order to improve the speed of the code, implicit algorithms (numerical methods with semi-implicit design and automatic time stepping) replaced old algorithms. Tests done to verify the new algorithm reveals that the execution speed is 3 to 30 times faster than in the previous algorithm. With information obtained from this code, engineers could study conditions in the reactors, their parametric behavior to obtain information for designing multiphase reactors**[27]**. The original method used in the old version of MFIX was developed by Harlow and Amsden in 1975 which was implemented in the K-FIX code. Later on, this method was used by Gidaspow and Ettehadieh in 1983 for describing gas solids flows at the Illinois Institute of Technology. Chemical processing and energy conversion units such as Fluid Catalytic Cracking (FCC) riser, usually use dense multiphase flow reactors[28].

For years, researchers (Laux and Johansen 1997 Fogt and Peric 1994, Spalding 1980) carried out studies in order to improve the code which was selected as a CFD commercial code. The theoretical and numerical essence of MFIX code is based on a hydrodynamic theory of fluidization, and many researchers (Davidson, 1961; Davidson and Harrison 1963; Jackson 1970, and others) have carried out studies on the development and application of the hydrodynamic model of this code for fluidization. In these studies hydrodynamic models were used for studying stability of fluidization and details of bubble motion. The equations governing this code will be presented in the following sections. To speed up this code, numerical methods with semi-implicit design and automatic time setting are used. The MFIX code has some limitations. Predictions presented by the model might not be accurate due to a variety of reasons such as incomplete formulation of the governing equations, lack of knowledge about constitutive relations, inadequate information on initial and boundary conditions, etc. In addition, users might not be skillful enough to simulate and analyze the results. To describe the theory of this hydrodynamic model, a series of governing equations, constitutive relations and initial and boundary conditions are used[27].

Geometry

For comparison purposes, the geometry that was chosen in this work has the same dimensions as was described by Jin and co-workers[30]. A schematic of the fluidized bed studied in this work is shown in Figure 1. Since for lower pressures the amount of particles transported by gas would significantly increase; hence, in this work the pressure was chosen to be higher than 10 bars. In this study, the gas inflow velocity and minimum fluidization velocity was changed from 20, 40 and 60 meters per second in the previous work to 5, 15 and 20 meters per second. Furthermore, the column size was changed from 30 × 15 cm to 45 × 15 cm to prevent particles from being carried by the gas.

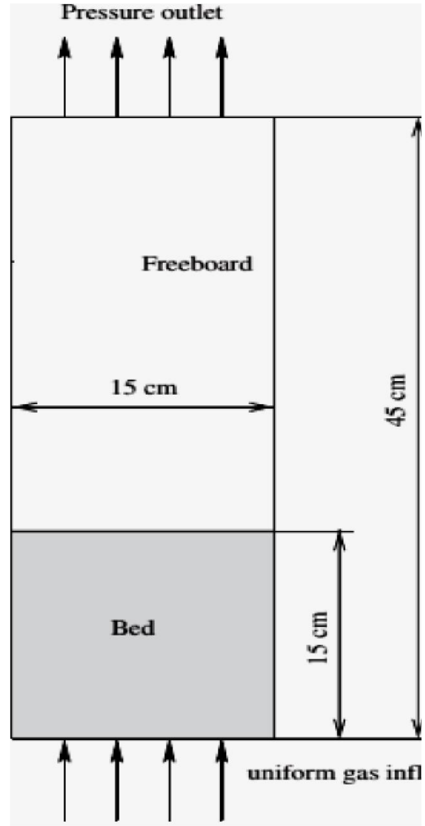

Figure 1 : Schematic of the fluidized bed studied in this work [30]

Initial and boundary conditions

In this work, the initial condition such as initial estimates for all computational cells and the solid volume fraction was introduced to the software by mfix.dat file manually. The velocity with uniform distribution of gas flow was considered as an inlet boundary condition for the lower end of the fluid bed. Furthermore, for the solid phase the inlet velocity was set at zero. For the bed outlet, the pressure boundary condition was chosen to be atmospheric pressure.

For the gas phase on the wall surface, no-slip boundary condition with zero velocity at the wall was considered; however, this was not the case for the solid

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phase. In this work, it was assumed that the vertical velocity of solid particles on the wall was zero and the tangential velocities of solid particles were the free-slip. Therefore, the no-slip boundary condition was used for the gas phase and the free-slip boundary condition for the solids at the wall.

Operating conditions

To study the segregation phenomenon for fluidized beds at high pressures, the density air was calculated from the following equation at atmospheric conditions:

$$\rho_{air} = 1.2 \times 10^{-3} \frac{gr}{cm^3} \qquad \textbf{(6)}$$

In this work, two solid particles of lithium and titanium have been employed. however, due to the restriction of software the mean density of particles have been utilized[31]. The mean density of particles was and particle diameter of lithium was 1.5 and titanium 2.25, 3.75 and 5.25 mm.

For the initial conditions, the of gas and solid phase in the bed was considered to be 0.41 and 0.295 respectively. In this study, the bed was modeled at pressures of 1 and 5 bar for the gas inlet velocity of and for 10, 20, 30 and 60 bar with gas inlet velocity of

RESULT AND DISCUSSIONS

Bed pressure drop

TABLE 1 shows the bed pressure drop at different operating pressures and particle size ratio. The results reveal that as the ratio of diameter of large to that of small particles increases, gas pressure drop in the bed increases accordingly. Furthermore, enhancement of the gas pressure drop in the bed increases the drag force applied by the gas to bed particles. Thus increasing the drag force balances the particles weight and fluidization occurs for the low gas velocity.

The above data are also plotted graphically as shown in Figure 2 where the horizontal and vertical axis are the pressure and the gas pressure drop in the bed at different pressures, respectively.

As Figure 2 demonstrates, increasing the pressure and particle size ratio would increases the pressure drop accordingly and hence reduces the minimum fluidization velocity of the bed particles.

Figure 3 shows the variation of the segregation value at a pressure of 1 bar and for different particle size ratios. As Figure 3 demonstrates and for a particle size ratio of 1.5 and for the velocity of , after 20 seconds

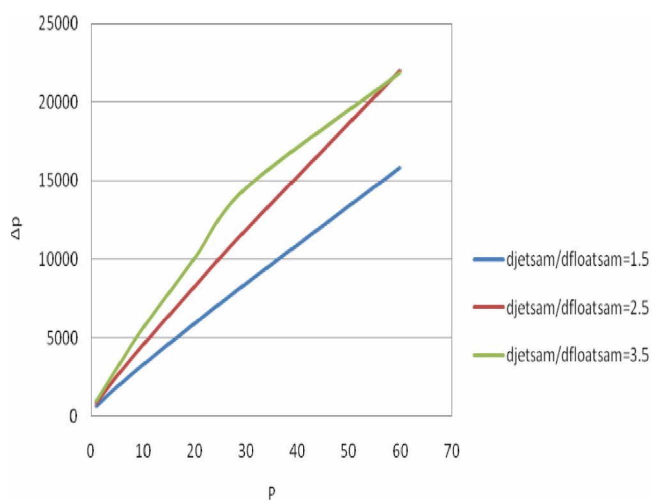

Figure 2 : Pressure drop variations with the operating pressure for different particle sizes and for the gas inlet velocity of 10 cm/s

TABLE 1 : The bed pressure drop at different operating pressures and particle size ratio

$^{djetsam}/_{dfloatsam} = 1.5$	$^{djetsam}/_{dfloatsam} = 2.5$	$^{djetsam}/_{dfloatsam} = 3.5$	P
$\Delta p = 684.97 \frac{dyn}{cm^2}$	$\Delta p = 865.283 \frac{dyn}{cm^2}$	$\Delta p = 1011.27 \frac{dyn}{cm^2}$	1bar
$\Delta p = 1899 \frac{dyn}{cm^2}$	$\Delta p = 2570.825 \frac{dyn}{cm^2}$	$\Delta p = 3082.6 \frac{dyn}{cm^2}$	5bar
$\Delta p = 3287 \frac{dyn}{cm^2}$	$\Delta p = 4524.1 \frac{dyn}{cm^2}$	$\Delta p = 5610.7 \frac{dyn}{cm^2}$	10bar
$\Delta p = 5917.4 \frac{dyn}{cm^2}$	$\Delta p = 8253.2 \frac{dyn}{cm^2}$	$\Delta p = 10049.2 \frac{dyn}{cm^2}$	20bar
$\Delta p = 8462 \frac{dyn}{cm^2}$	$\Delta p = 11870.4 \frac{dyn}{cm^2}$	$\Delta p = 14536.8 \frac{dyn}{cm^2}$	30bar
$\Delta p = 15836 \frac{dyn}{cm^2}$	$\Delta p = 22016.4 \frac{dyn}{cm^2}$	$\Delta p = 21877.4 \frac{dyn}{cm^2}$	60bar

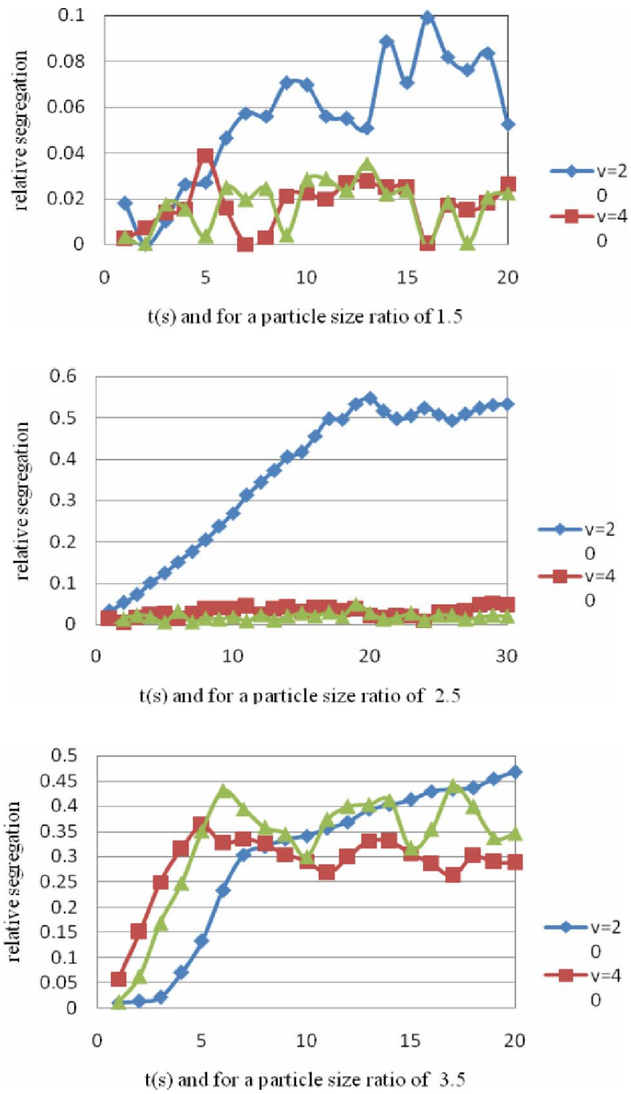

Figure 3 : Variation of the segregation value at a pressure of 1 bar and for a particle size ratio of 1.5, 2.5 and 3.5

the bed reaches the steady-state condition and the value of the segregation parameter approaches 0.09 which is close to zero and indicates almost complete mixing occurs in the bed. For the velocity of and from the start stability was observed in the bed and segregation parameters approaches 0.025 which indicates that complete mixing also occurs in bed. For the velocity of, from the start stability was observed in the bed and segregation parameters approaches 0.015 which indicates that perfect mixing occurs in bed.

As Figure 3 also demonstrates and for a particle size ratio of 2.5 and for velocity of , after 30 seconds a stability was observed in the bed and the segregation parameter approaches 0.63 which indicates a significant increase compared to previous cases.

Figure 3 also demonstrates that for a particle size ratio of 3.5 and for the velocity of , after 30 seconds stability was observed in the bed and the segregation parameter approaches 0.51. For the velocity of , after 20 seconds stability was also observed in the bed and complete particle segregation was achieved. For the velocity of and after 20 seconds the segregation approaches 0.3. As these results indicate for larger particle size ratios, an increase in the gas inlet velocity has no effect on the segregation pattern of particles.

Effects of pressure, gas inlet velocity and particle size ratio

To examine the effects of pressure on segregation, the segregation was plotted against the pressure for different operating pressures, as shown in Figure 4.

As shown in Figure 4, at particle size ratio of 1.5 an enhancement of pressure had no significant effect on the segregation value and hence complete mixing occurs in the bed. For particle size ratios larger than 2.5 and at velocity of , with an increase in the pressure the segregation decreases in the bed accordingly. However, at higher velocities the segregation increases with the enhancement of the pressure. The same trend was also observed in the particle size ratio of 3.5.

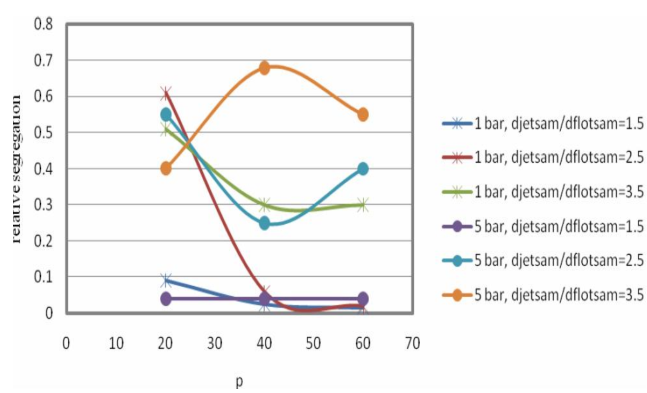

Figure 4 : Variation of the segregation at operating pressures of 1 and 5 bars

As Figure 5 for particle size ratio of 1.5 demonstrates, with an increase in the pressure pressure, segregation became more intense in bed. For gas inlet velocity of , the segregation in the bed decreases with an enhancement of pressure. However, with further increase of the velocity, the process got reversed. At higher gas inlet velocities, with an increase in pressure, the segregation also increases accordingly.

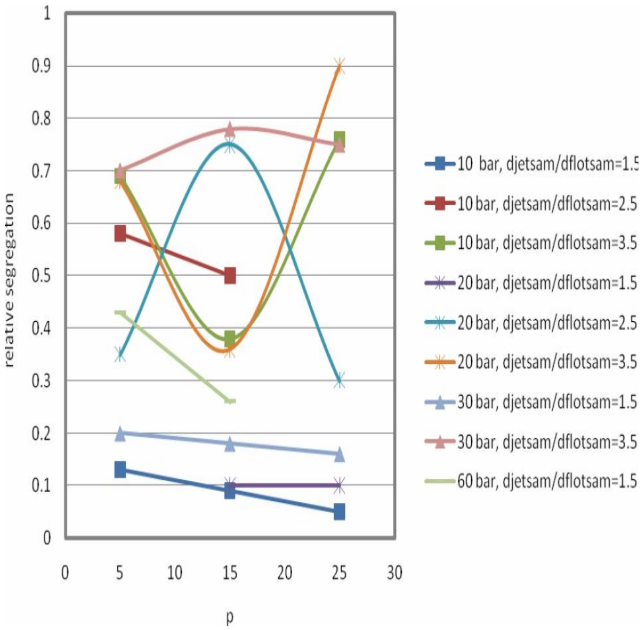

Figure 5 : Variation of the segregation at operating pressures of 10, 20, 30 and 60 bar

Figure 5. Variation of the segregation at operating pressures of 10, 20, 30 and 60 bar

For a particle size ratio of 3.5 and at pressures of 10 and 20 bar, except for the case of velocity of , an increase in the pressure did no significant effect on the rate of particle segregation. However, at gas inlet velocity of , an increase in the pressure caused higher segregation in the fluidized bed. At the pressure of 30 bars, only at gas inlet velocity of , the segregation was larger than similar cases at lower pressures.

In this work in order to investigate the simultaneous effect of particle size ratio and pressure on particle segregation in the bed, the segregation was plotted against the pressure (Figures 6 and 7). As Figure 6 demonstrates, at velocity of , with an increase in the pressure at all particle size ratios, the bed segregation decreases accordingly. The rate of changes in particle size ratio of 1.5 was very small and the difference became more evident with an enhancement of particle size ratios. Furthermore, at velocity of , with an increase in the pressure at all particle size ratios, the bed segregation also increases accordingly. At velocity of , with an increase in the pressure at all particle size ratios, the bed segregation also increases.

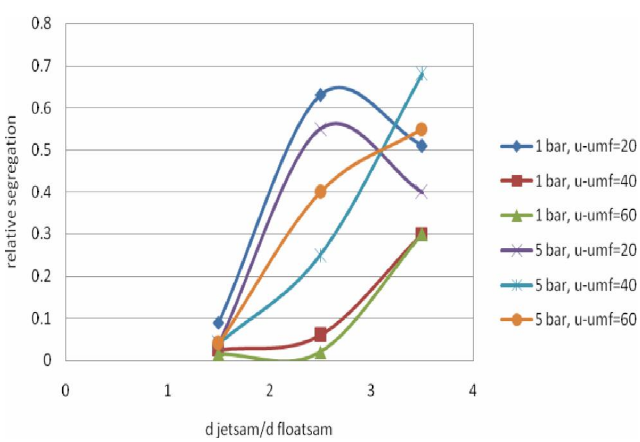

Figure 6 : Changes in segregation value at operating pressures of 1 and 5 bar based on particle size ratio

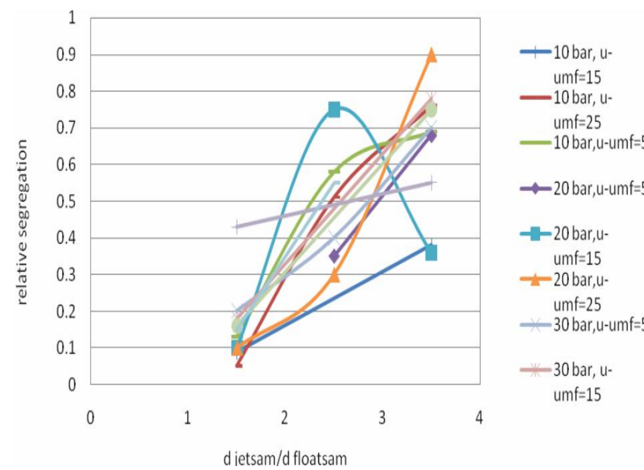

Figure 7 : Variation of the segregation at operating pressures of 10, 20, 30 and 60 bar

As Figure 7 demonstrates, at gas inlet velocity of , with an increase in the particle size ratio, the segregation also increases at all pressures; however, this increase was greater at lower pressures. At gas inlet velocity of , with an increase in particle size ratio, the segregation was also increased at pressures of 10 and 30 bar. However, at the pressure of 20 bars, it was initially increased and reached its maximum at a particle size ratio of 2.5 and then a decline in its values was observed. At gas inlet velocity of , with an increase in particle size ratio, the segregation value was also increased at all pressures..

Numerical validation

In order to validate the numerical results of present study, a comparative study has been made with the experimental data available in the literature as shown in Figure 8[30,36]. These comparisons have been made for the particle size ratios of 1.5 and 2.5 at a pressure of 1 bar and a velocity of 1.1 and 1.3 . Figure 8 shows that the results of this study are almost consistent with the experimental data available in the literature.

CONCLUSIONS

The hydrodynamics of gas-solid fluidized beds fluids are very complex in nature as the result of gravitational force between individual particles and the force between the particle and gas. Therefore, it was the aim of this work to examine the effect pressure, particle size and gas inlet velocity on mixing and segregation parameters in these beds. To obtain these objectives, a commercial computational fluid dynamics package namely MFIX were utilized and Paraview was also employed to analyze the data. The findings of the present study could be summarized as follows:

- An increase in the gas inlet velocity would cause almost complete mixing in the bed
- The effect of gas inlet velocity on the bed particle segregation was greater than that of particle size ratios
- Stability of the bed at particle size ratio of 1.5 could be attributed to the proximity of the particles
- The segregation at particle size ratio of 1.5 had little effect on the gas inlet velocity
- Particle segregation in the bed cold be justified with the enhancement of the particle size ratios
- With an increase in the gas inlet velocity, the bed particle segregation would decreases; however, the mixing increases
- For the particle size of 3.5 the segregation was higher at greater gas inlet velocities than at smaller gas inlet velocities which could be caused since the gas inlet velocity was approaching the minimum fluidization velocity.
- With the enhancement of the gas inlet velocity, a sharp increase was observed for the separation which was an indication that the gas inlet velocity was approaching the minimum fluidization velocity for larger particle

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