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FLUIDIZATION OF A BED OF SOLID PARTICLES IN A TWO DIMENSIONAL VERTICAL BOX

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ABSTRACT

Simulation of fluidization of a bed of solid particles in a two-dimensional box is performed using molecular dynamics methods by assuming that superposition of buoyant, gravitational, viscous, collision force will make the particle to move in two dimensions. Two different fluid type is used in this simulation, i.e., gas and liquid fluid. By increasing the fluid velocity from small to high, then minimum fluidization condition reached. As a result, fluidization of alumina particle with liquid fluid has a minimum fluidization velocity lower than gas fluid.

Keywords: alumina, fluid, fluidization, particle, simulation, velocity

INTRODUCTION

Granular material could be shifted into a different material phase for a certain period if the external force applied [1], i.e., by shaking the container [2], rotating the container [3], or flowing fluid into the material (particle) [4]. Fluid and particle interaction also exist in the phenomena of fluidization, which mainly used in a catalytic reactor for petroleum refining process [5]. The fluid flow phenomena in the catalytic reactor are sophisticated because of fluid and particle interaction to dissipate energy. Buchari et al. (2002) have established a numerical model for fluid flow in porous media [6].

Simulation of the fluidization process is essential to give more understanding of what happens in the fluidization and to obtain different results by changing the parameter. Simulation method commonly used for fluidization is Computational Fluid Dynamics (CFD), Molecular Dynamics (MD) [7], Discrete Element Method (DEM) [8], or by coupling two of these methods [9].

In this research, we run a simple simulation of fluidization by using Molecular Dynamics method. This research is to obtain the minimum fluidization velocity from a different type of fluid, i.e., gas and liquid.

METHOD

Particle Collision

The collision between two particles obey the Linear Momentum Conservation Law

$$m_i\vec{v}_i + m_j\vec{v}_j = m_i\vec{v}_i^{'} + m_j\vec{v}_j^{'}, \tag{1}$$

where m_i is a mass of the particle i, $\vec{v}_i$ is the velocity of the particle i, an apostrophe (‘) shows particle velocity after collision.

Dissipative energy is given by parameter e which is called the coefficient of restitution (CoR)

$$\vec{v}_i^{'} - \vec{v}_j^{'} = -e\left(\vec{v}_i - \vec{v}_j\right). \tag{2}$$

Equation (7) was used for a point mass; if the particle has any size then its time t and position $\vec{r}$ must be considered.

Modeling for a sized particle can be done by using a spring-mass model. Suppose we define a collision parameter named overlap ξ_{ij} as below

$$\xi_{ij} = \max\left(0, R_i + R_j - r_{ij}\right), \tag{3}$$

where

$$\begin{aligned} D_i &= 2R_i, \\ \vec{r}_{ij} &= \vec{r}_i - \vec{r}_j, \\ r_{ij} &= \left|\vec{r}_{ij}\right| = \sqrt{\vec{r}_{ij} \cdot \vec{r}_{ij}}, \\ \hat{r}_{ij} &= \frac{\vec{r}_{ij}}{r_{ij}}. \end{aligned} \tag{4}$$

The force act on the particle i due to collision with the particle j is given by

$$\vec{F}_{ij}^{N} = k_N \xi_{ij} + \gamma_N \dot{\xi}_{ij}, \tag{5}$$

where

$$\dot{\xi}_{ij} = \frac{d\xi_{ij}}{dx}, \tag{6}$$

k_N is spring constant and γ_N is its damping constant [10].

Gravitational Force

If the particles are near the earth surface, gravitational force attracted the particle i

$$\vec{F}_i^{G} = m_i \vec{g}_i = \rho_i V_i g \hat{g}, \tag{7}$$

where $\vec{g}$ is gravitational acceleration.

Buoyancy Force

If fluid exists around the particles, then buoyancy force exists

$$\vec{F}_i^{\rho} = -\rho_f g V_i \hat{g}, \tag{8}$$

where $\hat{g}$ is $\frac{\vec{g}}{g}$ and g obtained from Equation (11).

Drag Force

If fluid move with velocity $\vec{v}_f$, then every particle will experience a drag force

$$\vec{F}_i^{\mu} = -6\pi\mu_f R_i \left(\vec{v}_i - \vec{v}_f\right). \tag{9}$$

Newton's 2nd Law

If the system has N particles and M walls, then the total force acting on a particle i is given by

$$\sum \vec{F}_i = \vec{F}_i^{G} + \vec{F}_i^{\rho} + \vec{F}_i^{\mu} + \sum_{j \neq i}^{N} \vec{F}_{ij}^{N} + \sum_{j=1}^{M} \vec{F}_{ij}^{N}, \tag{10}$$

thus by Newton's 2nd law, we can obtain acceleration of a particle i as follow

$$\sum \vec{F}_i = m_i \vec{a}_i,$$
$$\vec{a}_i = \frac{1}{m_i}\left(\vec{F}_i^{G} + \vec{F}_i^{\rho} + \vec{F}_i^{\mu} + \sum_{j \neq i}^{N} \vec{F}_{ij}^{N} + \sum_{j=1}^{M} \vec{F}_{ij}^{N} \right). \quad (11)$$

Euler's Integration

By using Euler's algorithm, position and velocity of each particle can be obtained as follow, respectively

$$\vec{v}_i\left(t+\Delta t\right) = \vec{v}_i\left(t\right) + \vec{a}_i(t)\Delta t,$$
$$\vec{r}_i\left(t+\Delta t\right) = \vec{r}_i\left(t\right) + \vec{v}_i(t)\Delta t. \quad (12)$$

Flowchart Diagram

The whole process in the simulation is given in FIGURE 1.

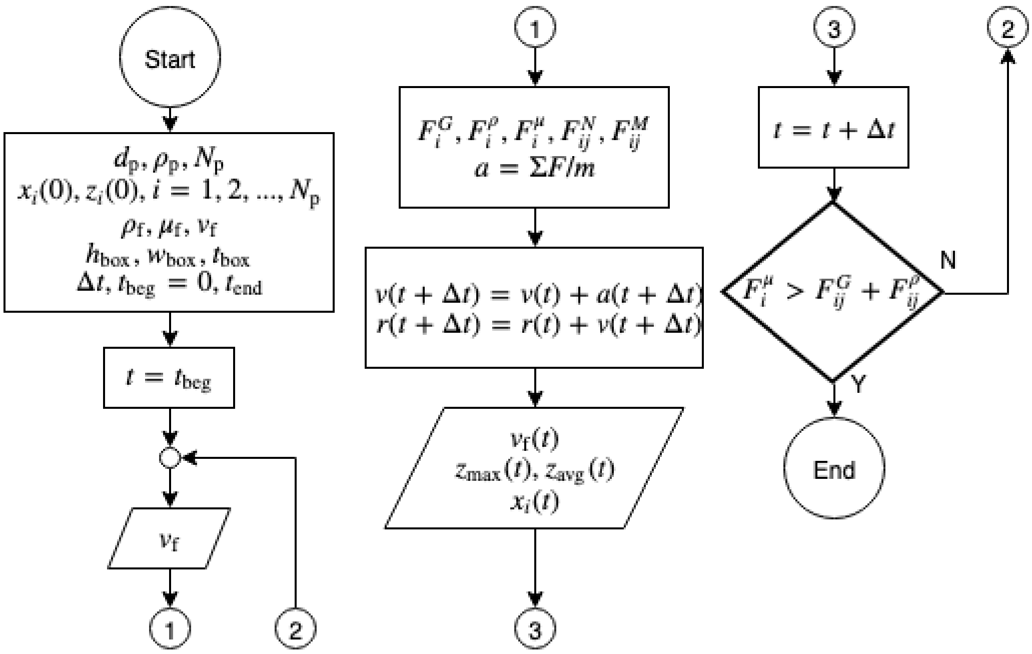


FIGURE 1. Flowchart diagram of simulation of the fluidization process in a two-dimensional vertical box.

RESULT AND DISCUSSION

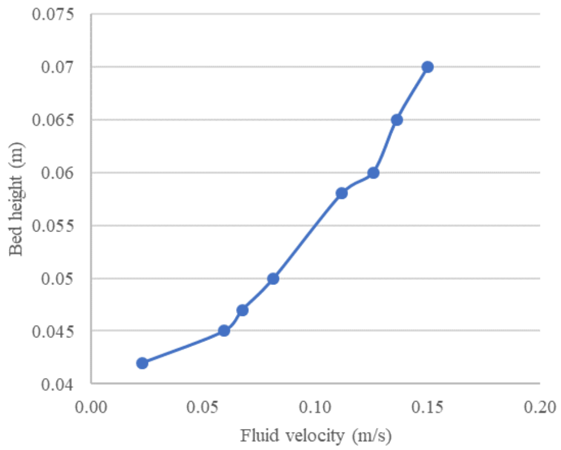
Input parameter which used in this simulation is given by TABLE 1. In the experiment, this particle density value represents alumina particle, with a diameter in the order of 10^{-4}. Due to our computer limitation, we made scaling for diameter in the simulation to the order of 10^{-2}. We use two different fluid types, i.e., liquid and gas. Each fluid type has different viscosity and density value which can be seen from the table. Fluid velocity starts from 0 m/s to 100 m/s by increasing 10 m/s until the minimum fluidization condition is reached.

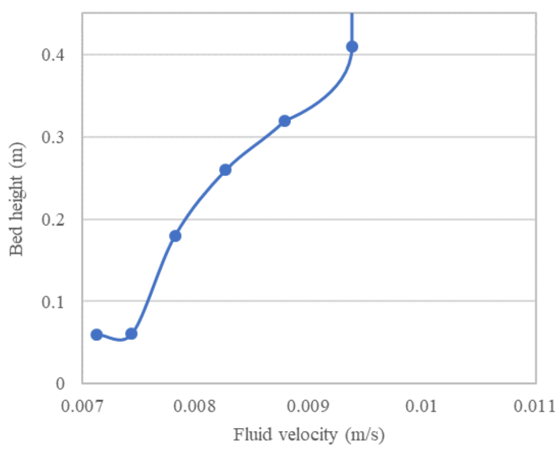
TABLE 1. Input parameter used in the simulation.

Parameter	Value	Units	Explanation
d_p	0.01	m	Particle diameter
ρ_p	2000	kg.m^{-3}	Particle density
N_p	90	-	Number of particles
ρ_f	1000, 1.1644	kg.m^{-3}	Liquid, gas fluid density
μ_f	1.0016×10^{-3}, 1.85×10^{-5}	Pa.s	Liquid, gas fluid viscosity
v_f	0, 10, …,100	m.s^{-1}	Fluid velocity
$h_{box}, w_{box}, t_{box}$	0.4, 0.15, 0.15	m	Box height, width, thickness
Δt	0.001	s	Time step
t_{beg}, t_{end}	0, 100	s	Begin, end time

Experimental Result

FIGURE 2 shows the experimental result for fluidization of alumina particle using (a) gas and (b) liquid fluid. This experimental result collected from the Chemical Engineering Department, Institut Teknologi Bandung, as an undergraduate student's Instructional Laboratory report. In gas fluid, alumina particle fluidized when fluid velocity is higher than 0.05 m/s and spouted when fluid velocity is higher than 0.10 m/s. In liquid fluid, alumina particle fluidized when fluid velocity is higher than 0.0075 m/s, but entrained when fluid velocity is higher than 0.009 m/s.



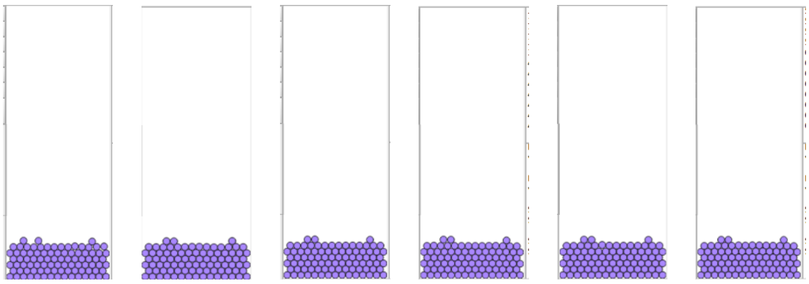


(a) (b)

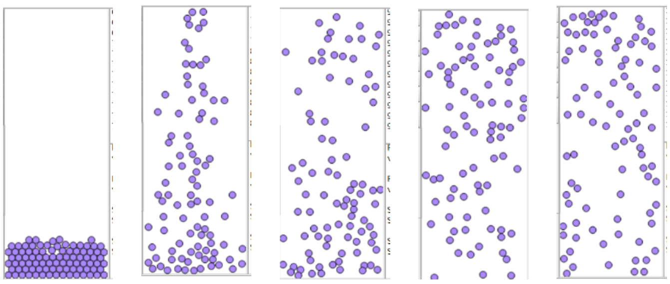
FIGURE 2. Experimental result for fluidization of alumina particle with (a) gas fluid and (b) liquid fluid.

Simulation Result

Simulation result consists of particle motion, average bed height, and maximum bed height, given by FIGURE 3 and 4 for gas fluid and FIGURE 5 and 6 for liquid fluid. For gas fluid, alumina particle remains in its position when fluid velocity is below 70 m/s, and above that alumina particle start to blow up. So, we consider this as minimum fluidization velocity for gas fluid. For liquid fluid, alumina particle remains in its position when fluid velocity is below 60 m/s, and above that alumina particle start to blow up. So, we consider this as minimum fluidization velocity for liquid fluid. The motion of particles observed here is more random than in the experiment, and also it is difficult to see whether a bubble is formed. In the experiment, we use maximum bed height rather than average bed height.

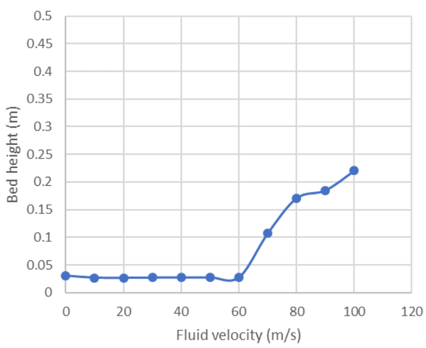


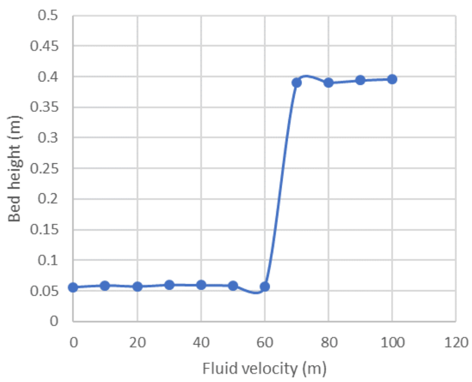
(a) (b) (c) (d) (e) (f)



(g) (h) (i) (j) (k)

FIGURE 3. Particle motion in simulation of fluidization process using gas fluid with fluid velocity increase: (a) 0 m/s, (b) 10 m/s, (c) 20 m/s, (d) 30 m/s, (e) 40 m/s, (f) 50 m/s, (g) 60 m/s, (h) 70 m/s, (i) 80 m/s, (j) 90 m/s, and (k) 100 m/s.





(a) (b)

FIGURE 4. Average and maximum bed height in a simulation of the fluidization process using gas fluid.

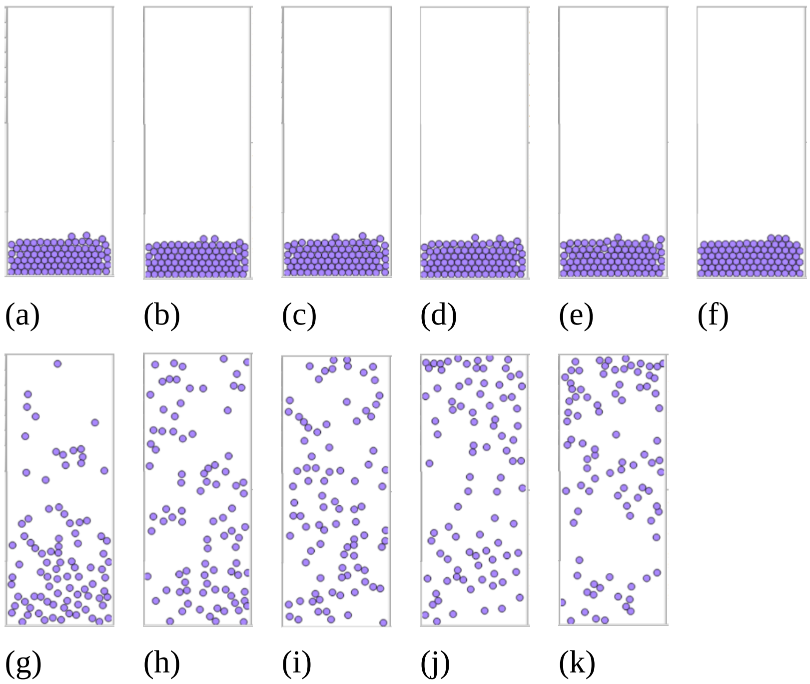


FIGURE 5. Particle motion in a simulation of fluidization process using liquid fluid with fluid velocity increase: (a) 0 m/s, (b) 10 m/s, (c) 20 m/s, (d) 30 m/s, (e) 40 m/s, (f) 50 m/s, (g) 60 m/s, (h) 70 m/s, (i) 80 m/s, (j) 90 m/s, and (k) 100 m/s.

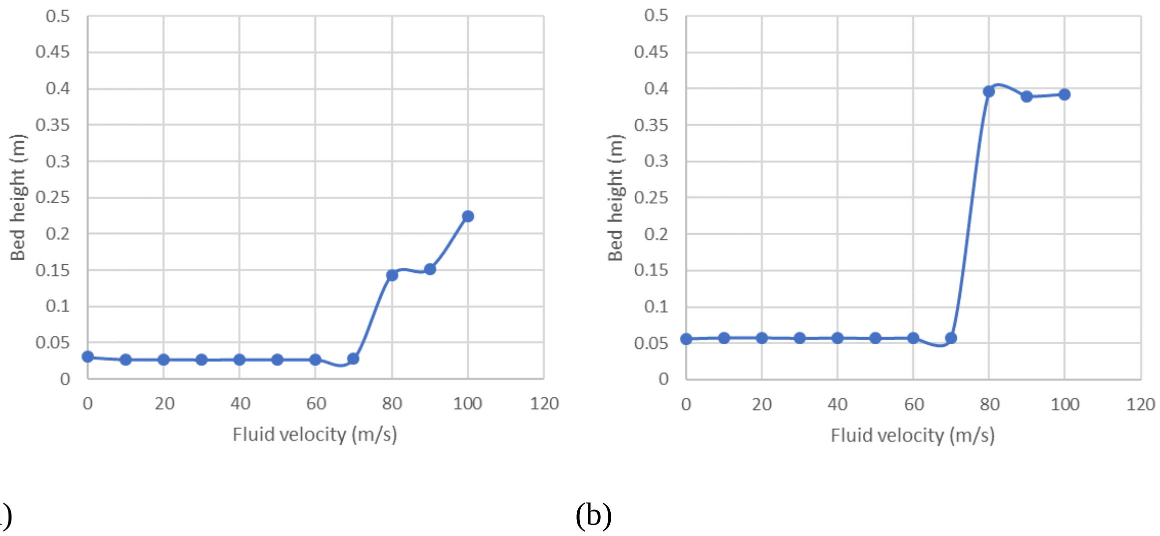


FIGURE 6. Average and maximum bed height in a simulation of the fluidization process using liquid fluid.

CONCLUSION

From this research, simulation of fluidization has been conducted for alumina particle with both gas and fluid liquid. As the results, we can conclude that minimum fluidization velocity for alumina particle is lower with liquid fluid than with gas fluid. Qualitatively, the simulation agreed with the experimental result.

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