Two Dimensional Simulation of Deposited Polydisperse Particles

Ni’matur Rohmah\textsuperscript{1}, Moh. Hasan\textsuperscript{2}, Alfian Futuhul Hadi\textsuperscript{3}

\textsuperscript{1,2,3}Department of Mathematics, Faculty of Mathematics and Natural Sciences, Jember University, Indonesia
\textsuperscript{1}Email: justniksma20@gmail.com, \textsuperscript{2}Email: hasan.fnipa@unej.ac.id

Abstract—This research aims to study dynamic and static conditions aspect deposition of particles. Simulation applies Granular Dynamics model to describe contact forces simultaneously. The movement of particles forms a trajectory. The trajectory of particles resolved by Gear Predictor-Corrector method. Simulation involved a variation of the standard deviation value of particle diversity in two dimensional simulation of polydisperse particles. The results of simulation are images of deposition process for every time iteration until the pile of particles in static condition. Conclusion is the smaller standard deviation value, cause the greater angle of repose of pile, and otherwise the greater standard deviation value, cause the smaller angle of repose of pile. So, the standard deviation size diversity of particles is inversely proportional height and slope of forming pile structure.

Keywords—Deposition, Granular Dynamics, Polydisperse, Standard Deviation

1. INTRODUCTION

Granular particles are related to daily life, such as sand, stones, grain of rice, beans, sugar, potatoes, and capsules. Granular particles behavior are unique. They can be like a solid, liquid, and gas. It was involved with external condition [3]. Particles dynamics are study of forces and motion that occur of particles. Forces of movement particles are normal force, tangential force, and gravity force. A lot of treatments from particle dynamics is deposition. Particles deposition are dropping grains into free surface, a pile is formed. The pile almost forms a triangular with irregular surface.

Particles deposition has been studied force of collision model with stick and slip phenomenon. It result of multiple transition phenomenon at behavior particle during deposition process. Multiple transition is from statics to dynamics and dynamics to statics. The simulation use monodisperse particle for simple model [6]. Not only monodisperse particle, but also we can simulated to find out the particle dynamics with different size, it call polydisperse particles. For polydisperse particles has discussed on [1] and [4]. On reference [4], it has discussed polydisperse frictional particles packing. The conditional probability distributions of particle overlaps are determined by molecular dynamics simulations. It depends on polydispersity and friction coefficient.

On the other hand, this deposition process involves many particles to be simulated. The particles which are simulated statistically are considered as data, which in this process can be observed the distribution of particles that occur. Discussion of particles within large numbers refers to analysis of particle size distribution. It is used to observe, control, and analyze large quantities of industrial materials [3]. For another type of particles namely polydisperse hard sphere, On reference [1], It has discussed the comparison between particle size distribution with gauss distribution and result experiment of Transmission Electron Microscopy (TEM) method. They also did variation on standard deviations to determine of particles scattering.

Based on previous researches, in this paper discuss polydisperse particles deposition with variation on standard deviations values. The purpose of writing is to find out the dynamic and static conditions result of dropping particle by providing variations in standard deviation.

II. RESEARCH METHODS

The first step of simulation was determining collision criteria. Collisions between particles occur when the distance between the two circles is less than the sum of the radius of the two particles. Formulation of collision criteria for polydisperse particles the number of the two radius is formulated with \( r_1 + r_2 \) because the size of radius particles is different. So, collision criteria for circular particles with heterogeneous diameter sizes formulated by \( \varphi_{ij} = d_{ij} - (r_1 + r_j) \). It given criteria \( \varphi_{ij} < 0 \) is distance of center point of two particles, \( r_1 \) radius of particle i-th and \( r_j \) radius of particle j-th. While the criteria of particle collision with media, for polydisperse particles \( \varphi_{zi} \) formulated by \( \varphi_{zi} = \)
It given criteria \( \varphi_{zi} < 0 \). \( z_i \) is the position of particle in vertical direction. The second step is simulation with Digital Visual Fortran software and interpretation of results. The number of particles simulated \( N = 900 \) particles by giving three different colors namely red, yellow, and green for each of the 300 particles. Particles dropped from height \( h = 3 \text{ m} \), normal and tangential velocity \( v_n = v_t = 5 \times 10^{-3} \text{ ms}^{-1} \), it is assumed that all particles have the same mass \( m = 0.05 \text{ kg} \) although the diameter is different, elasticity constants in the normal and tangential directions \( k_n = k_t = 10^5 \text{ kg s}^{-2} \), stick velocity \( \varepsilon = 10^{-2} \text{ ms}^{-1} \), time step \( \Delta t = 10^{-5} \text{s} \), coefficients of dynamic friction \( \mu_d = 0.3 \), and coefficients of statics friction \( \mu_s = 0.6 \). The value of normal damping constant \( \gamma_n \) has given by Equation 1

\[
y_{\text{n-crit}} = 2 \sqrt{m.k_n}
\]

given parameter values as known previously \( y_{\text{n-crit}} \approx 140 \). Because \( k_n = k_t \), so

\[
y_{\text{t-crit}} = 2 \sqrt{m.k_t} = y_{\text{n-crit}},
\]

where \( y_{\text{n-crit}} \) critical normal damping constant and \( y_{\text{t-crit}} \) is critical tangential damping constant. Normal damping constant has a half value of \( y_{\text{n-crit}} \), whereas tangential damping constant has equal with \( y_{\text{t-crit}} \). Given \( y_n = 0.5 \) and \( y_{\text{n-crit}} \) equal with coefficient of restitution value (\( \psi \)) is 0.3. Described \( \psi \) in Equation 2

\[
\psi = \exp \left( -\frac{\gamma_n}{\omega} \left( \pi - 2 \arctan \left( \frac{y_n}{\omega} \right) \right) \right)
\]

with \( \omega = (4mk_t - \gamma_n^2)^{1/2} \) [5].

The random number of diameter particles has obtained the largest of diameter particles i.e.0.121 m. Collision of two particles cause particles bounce to unexpected direction. So we can set the time collision of two particles to avoid it. For simple program, we use the largest particles for determine safest distance of particles. So, for the smaller particles are follow it. Formulated of mileage free fall particle is

\[
s = \frac{1}{2} g t^2 + v_0 t \]

where \( g \) is acceleration of gravity (9.81 m/s\(^2\)), \( t \) is time, and \( v_0 \) is initial velocity of particles. If \( s \) equals the largest of diameter particles and \( f_{\text{n-crit}} = n.\Delta \text{ with } \Delta t = 10^{-5} \) then based on Equation (3) obtain \( n \approx 15,706 \). We choose distances between first particle falling in order not to collide with the second particle must fall after 15,800-th iteration. The interpretation of the results dynamically is seen from a collection of images made by the movie with the movie maker software and the final image results in a pile in a static condition.

Random particle diameters are generated using the Linear Congruent Generator (LGC) method, which is a randomly generated random number generation method using the gauss function. Normal distribution has two parameters namely mean \( \mu \) and standard deviation \( \sigma \). If we give the same mean but different standard deviations, curve are centered at exactly the same position on the horizontal axis, but the curve with the larger standard deviation is lower and spreads out farther [8]. Particle velocity is defined in the \( x \)-axis direction, whereas in the \( z \)-axis direction it is made zero so that all particles are given a velocity that has a direction. Although the diameter particle is random number, but it is assumed that all particle have the same mass. The purpose of that assumption is to focus of heterogeneity particles.

Trajectory particles determined by using the Predictor-Corrector method which is specifically using the Gear Predictor-corrector method. As for the steps are prediction, evaluation, and correction stages [7]. Prediction stage is used to predict the initial position value of a particle, velocity, acceleration, third derivative, and fourth derivative of the particle position. Evaluation stage contains steps for calculating each force involved on all particles during the dynamic process, so that they can determine the possibility of particles colliding with each other. The Correction stage is the last step in Gear method. The acceleration of the correction is obtained from the force that has been obtained from the evaluation process divided by the mass of the particle, so that the values of position, velocity, acceleration, third derivative, and fourth derivative of the particle position are better.

The force calculation starts with calculating the possibility of particles colliding with each other. Two colliding particles have their own criteria which have been explained previously. Other particles that are within a range of these particles are called neighbors, while particles that have the possibility to collide are called partners. The core program also defines particles that are more likely to collide, called neighbor list. It is efficient the running program by not needing to do calculations on \( n - 1 \) other particles. In addition to calculating the probability of collisions between particles, it is also examined the possibility of collisions of particles with the medium in which the particles are dropped.

If particle qualify the collision criteria with a particle then the particle will be save as a partner of particle i, then the normal force \( f_n \) is calculated between the two particles by first calculating the relative velocity, relative acceleration, and the unit vector in the normal direction using Equation (4)

\[
f_n = -(k_n \delta_n + \gamma_n v_n),
\]

where \( \delta_n \) is the relative displacement in the normal direction, \( v_n \) is the relative velocity in the normal
direction, $k_n$ is the normal elastic constant, and $\gamma_n$ is the normal damping constant. Then the particle displacement and relative velocity in the tangential direction are calculated to get the friction between the two particles using Equation (5)

$$f_i = \begin{cases} (k_t \delta_t + \gamma_t v_t), & |v_t| \leq \varepsilon \text{ (static friction)} \\ -v_t \mu_d f_n, & |v_t| > \varepsilon \text{ (dynamic friction)} \end{cases}$$

where $f_i$ is tangential force, $k_t$ is the tangential spring constant, $\delta_t = \int_0^t v_t(\tau) \, d\tau$, i.e. the total tangential displacement during time $t - t_0$, $v_t$ and $\nu_t$ is the relative tangential velocity and vector shape, $\mu_d$ is the dynamic friction coefficient, $\gamma_t$ is the tangential damping coefficient, and $\varepsilon$ is speed threshold [5].

Tangential and normal force are summed to get the resultant force received by the particle. This process takes place at any time $dt$ until all particles dropped before particle $i$ are examined against the collision criteria for particle $i$ using Equation (6)

$$f = mg + \sum c_i$$

where $f$ is the contact force between particles, $m$ is the mass of the particle, $g$ is the gravitational force of the earth $(9.81 \text{ m/s}^2)$, and $c_i$ is the contact force on the $i$-th particle [5]. If particle qualify collision criteria with the medium, the normal and tangential forces of the particle are calculated like collision with other particles. These forces are added with the previous collision forces also. Another force involved on particles deposition is gravity. This force works on each particle and reduce force that leads to tangential direction. And so on until all particles have been dropped and all particles have remained or until they reach a predetermined step limit.

III. RESULT AND DISCUSSION

3.1 Dynamics and final structure of pile

These observations describe the dynamic condition of particles deposition. It was used to produce movie, consisting of a series consecutive figures of the pile configuration. Based on movie, the first particles dropped will hit the medium directly. Then followed by particles that fall afterwards, it will hit particles that have fallen first so that the particles accumulate with each other.

The particles dropped earlier being covered by layers of drop later, and piling up. Furthermore, the particles dropped may not replace the earlier particle, but it go down through the edge of the pile directly and avalanches surface of the pile has been passed. After a long time, the pile is formed higher and parts of pile that avalanche are the edges. It is caused by the displacement of particles that fall later the pile is formed to obtain a shorter pile than the particles dropped earlier. So the force that occurs on particle cannot overthrow the pile has formed. Particle movement continues although all particles have been dropped. It caused by simultaneous movement of dropping particles, so that some of the particles are still in the neighbor list internal landside until each particles at stable position. Result of simulation is stable pile of polydisperse particles deposition given by Fig.1

![Fig. 1 Stable pile of polydisperse particles deposition](image)

Based on Figure 1, small particles are more dominant in the middle of pile. This results also caused distribution of large-sized particles dominate the outside of pile, whereas the middle of pile is dominated by small-sized particles that push large particles into the outer side. The formed of pile is tends to be sloping, due to smaller sized particles entering between slits the larger sized particles.

The pile can be estimated as isosceles triangle. It has an almost symmetrical triangular shape with an irregular surface. So, angle of repose is calculated by Equation (7)

$$\alpha = \tan^{-1}\left(\frac{2h}{b}\right)$$

with $h$ the height of triangle and $b$ is the base of triangle. The height and base of triangle given by Equations below

$$h = 3\gamma_c$$

$$b = \frac{24}{N} \sum_{i=1}^{N} (x_i - x_c)^2$$

$$\gamma_c = \frac{1}{N} \sum_{i=1}^{N} y_i, \text{ and } x_c = \frac{1}{N} \sum_{i=1}^{N} x_i$$

$x_c$ and $y_c$ are the coordinates of particles centre, $x$ and $y$ are the centre of mass of the pile and the triangle [6]. So, the stable pile of polydisperse particles deposition as Figure 1 was obtained angle of repose 27.45°.

3.2 Variation of standard deviation values

Variation of standard deviation is given to find out the dynamic and static conditions result of dropping particles. It presented in Table 1.
Table 1. Comparison of the results simulation with variation standard deviation values

| Standard deviation $\sigma$ | Angle of Repose ($^\circ$) | Image |
|-----------------------------|-----------------------------|-------|
| $10^{-3}$                   | 39.6                        |       |
| $10^{-2}$                   | 37.2                        |       |
| $10^{-1}$                   | 27.45                       |       |

Based on the Table 1, the smaller standard deviation value, cause the greater angle of repose of pile, and otherwise the greater standard deviation value, cause the smaller angle of repose of pile. So it can be concluded that the standard deviation values of particles diversity is inversely proportional to the angle of repose occurring on the pile.

Associate results between simulation of deposition polydisperse particle and statistical approach with variation of standard deviation values, they have the same behavior. As a proof this statement, it given explanation with Figure 3, difference between the stable pile of monodisperse and polydisperse particles deposition.

![Image](image1.png)

Fig. 3 (a) Stable pile of monodisperse particles deposition, (b) Stable pile of polydisperse particles deposition

The form of pile results deposition monodisperse particles is higher than result of polydisperse particles. The angle of repose monodisperse particles is $52.85^\circ$ and for polydisperse particle is $27.45^\circ$.

IV. CONCLUSION

The results of deposition polydisperse particle simulation are form of pile lower than monodisperse particle deposition. The variation of standard deviation values in the program gives the fact that the physical concept of deposition of heterogeneous particles forms a pile that mathematically resembles the concept of a normal distribution curve. The standard deviation of the particle size diversity is inversely proportional to the height and slope of the formed pile structure.

REFERENCES

[1] E. Zacarelli, S.M. Liddle, and Wilson, C.K. (2015). On Polydispersity and the Hard Sphere Glass Transition. Journal Soft Matter : Royal Society of Chemistry, Hal: 342-330.
[2] G.H. Beaucage, H.K. Kammler, and S.E. Pratinis (2004). Particle size distributions from small angle scattering using global scattering functions. Journal of Applied Cristallography. Volume 37. Issue 4.
[3] H.M. Jaeger, S.R. Nagel, and R.P. Behringer (1996). Granular Solids, Liquids, and Gases. Rev. Mod. Phys., Vol. 68, No. 4, pp. 1259-1273.
[4] K. Saitoh, V. Magnanimo, and S. Luding (2015). A Master Equation for Force Distributions in Polydisperse Frictional Particles. Proceeding of the 4th International Conference on Particle-Based Methods-Fundamentals and Application, PARTICLES. Pages:1028-1039, Number :12.
[5] M. Hasan (2003). Deposition and Shaking of Dry Granular Piles: A Granular Dynamics Model for Reversible Transitions Between Stick and Slip Contact. PhD Thesis, Wageningen University, Netherlands.
[6] M. Hasan and J.H.J Van Opheusden (2007). A Model for Static and Dynamic Phenomena in Deposition Processes. J. Indones. Math. Soc. (MIHMI), Vol. 13, No. 2. pp. 173(189).
[7] M.P. Allen and D.J. Tildesley (1999). Computer Simulation of Liquids. England: Oxford University Press.
[8] R.E. Walpole, R.H. Myers, S.L. Myers, and K. Ye (2002). Probability and Statistics for Engineers and Scientists. Prentice Hall, Inc.