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Simulation of Heterogeneous Particle Deposition using Digital Visual Fortran

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Abstract—Granular particles have unique behaviour because it can behave like solids, liquids, and gaseous subtances. So, it is necessary to discuss the dynamics of these particles. Dynamical particles involve normal force, tangential force, and gravity force. Deposition is dropping particles at a medium, it produces a pile of particles. First step of simulation is assigned collision criteria. Next step is simulation using digital visual Fortran software and the final step is to analyze it. Based on simulation, dynamic behavior of particles is seen through on video created by assembling images of simulation result. The largest particles are fallen spread to underlying medium then followed by smaller particles. It fallen on center of pile until particles below bears a much heavier than the mass of particles. The smaller particles on center of pile pushes at the bottom and it makes cavity. As a result, the pile seems to have two peaks on static condition

Keywords— Deposition, Granular particles, Simulation, Fortran.

I. INTRODUCTION

Granular particles are closely related to everyday life, such as sand, stones, grains of rice, nuts, sugar, potatoes, and capsules. The behavior of granular particles is unique. They can be solid, liquid, and gas. It is related to external conditions [1,2]. Particle dynamics studies the force and motion that occur in particles [3]. The moving particle forces are the normal force, the tangential force, and the gravitational force [4].

One of the treatments related to particle dynamics is particle deposition. Particle deposition is the process of dropping particles onto a flat surface and forming them [5,6]. The piles are almost triangular with irregular surfaces. The deposition of particles causes the particles to collide with each other. This is caused by the double transition phenomenon in the behavior of the particles during the deposition process. Multiple transitions are from static to dynamic and dynamic to static [5].

Precipitation of particles in previous studies used monodisperse particles. Not only monodisperse particles, but we can simulate to find out the dynamics of particles with different sizes [7]. These are called polydisperse particles. Polydisperse particles mean the diversity of particles, such as particle size and shape [8,9]. We have studied a simulation of deposition of polydisperse particles that varies the value of the standard deviation with respect to the effect on the shape of the pile. The result showed that the standard deviation variation in particle diameter size was inversely proportional to the height and angle of inclination of the pile structure formed [10].

Based on previous research, this article discusses the deposition of polydisperse particles by sorting the particles from largest to smallest in diameter. If you want a truly realistic particle dynamics model, you need a complex and complicated model. Therefore, this study uses the assumption that the simulated particles are circular in shape with heterogeneous sizes, the particles fall on a flat surface, and the particles have hard properties. So that when it collides with other particles, it does not change shape.

II. METHODS

Figure 1 is the method used in this study to simulate heterogeneous particle deposition. Basically, there are three stages as follows:

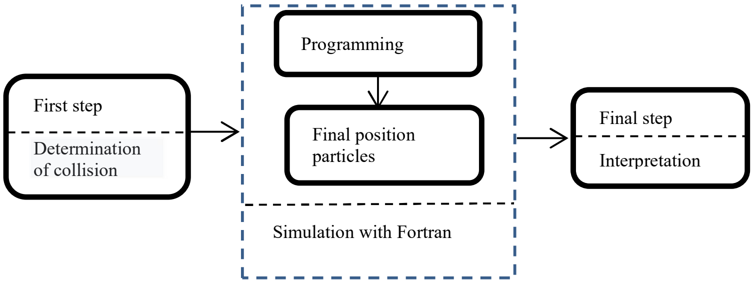


Fig. 1. Research scheme

A. Determination of collision criteria

Particle behavior is influenced by the behavior of other particles that are equally moving, thus allowing collisions to occur. Two colliding particles are illustrated in Figure 2. The movement of large numbers of particles allows a particle to collide with more than one particle depending on the direction and distance between the particles. The position of a particle per unit time is affected by the speed and acceleration of the particle's motion thus forming a trajectory.

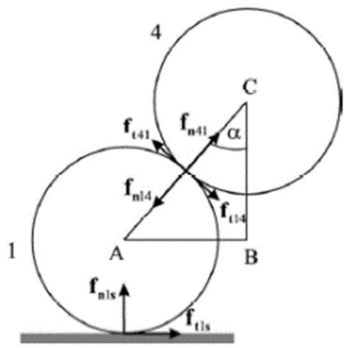


Fig. 2. Force acting on two homogeneous particles colliding
Source: (Hasan, 2003).

Particles that have the potential to collide are not determined by the distance between the particles, but by the direction of motion of the particles. The criteria for the potential collision can be formulated as $v_{ij}.rn_{ij} < 0$ [7]. The complete system built in this simulation is illustrated in Figure 3, particles dropped at a height of h_0 are heterogeneous particles and these particles will form a mound.

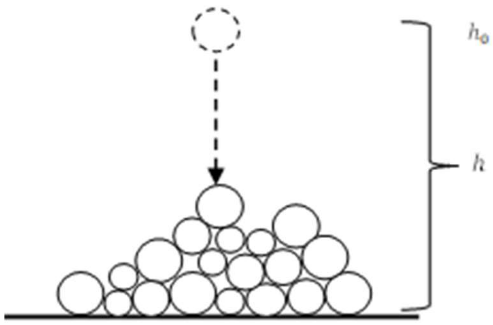


Fig. 3. Illustration of research system

B. Simulation with Fortran

Making software to simulate particle dynamics models in particle deposition processes with heterogeneous particle size variations using Digital Visual Fortran software [11,12]. These steps include defining variables and parameters, calculating the forces acting on the system when static and dynamic, numerical solutions using the Predictor-Corrector method [13] and printing in the form of images in the form of postscript files for each particle movement per unit of time. The final structure of the mound resulting from heterogeneous particle deposition can be observed from the static conditions and dynamic conditions can be observed through the movies compiled from these images. The fixed parameters used in the simulation are presented in Table 1.

Table 1. Value of parameter

Parameter	**Value**
$k_n = k_t$	$10^5 kgs^{-2}$
$v_n = v_t$	$5x10^{-3}$
m	0.05 kg
g	$9.81\ ms^{-2}$
N	900
h	3 m
$\gamma_n = \gamma_t$	0.5
$\mu_s = \mu_d$	0.4

where n is the number of particles, k_n and k_t normal and tangential elasticity constants, v_n and v_t are the normal and tangential particle velocities, m is mass, ε is the threshold velocity, Δt time step, and γ_n and γ_t are normal and tangential inertia. Furthermore, the simulation is arranged in descending order of the diameter of the dropped particles. Sorting the diameter of the particle size resulting from random number generation is sorted using Microsoft Excel for descending sorting [14,15]. The results obtained from the simulation, namely the shape of the mounds in static conditions and dynamic conditions can be seen from the movies made.

C. Interpretation of Results

The results of this simulation software are in the form of images of particle positions per unit time until the final movement, namely in the form of mounds and the dynamics of their deposition, can be seen through a movie made from the series of images. So that from the movie it can be used to find out the final structure of the particle mound by sorting the particle sizes in descending order during the dropping process

II. RESULTS

A. Determination of collision criteria

If suppose that r_1 is the radius of the first particle and r_2 is the radius of the second particle, then the sum of the radii of the two heterogeneous particles is formulated by $r_1 + r_2$. Collisions between particles occur when the distance between the two particles is less than the sum of the radii of the two particles. Suppose d is the distance between the two center points of the circle, then the condition of the heterogeneous particles is in a collision condition between the particles presented in Figure 4 below:

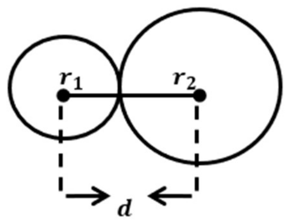


Fig. 4. Illustration of collisions between heterogeneous particles

Based on this illustration, collisions between heterogeneous particles can be formulated as follows:

$$\varphi_{ij} = d_{ij} - (r_i + r_j) \tag{1}$$

where φ_{ij} is the difference between the distance between the two particle centers and the particle diameter. Equation (1) is used to detect collisions that occur, so that there are no collisions between particles, a condition is given $\varphi_{ij} < 0$. In addition to collisions between particles, the criteria for collisions between particles and the medium in which the particles are dropped must also be determined. The collision between the particle and the medium occurs if the distance from the center of the particle to the medium is less than the radius of the particle which is formulated as follows:

$$\varphi_{zi} = z_i - r_i, \tag{2}$$

where φ_{zi} is the difference between the distance from the center of the particle to the media and the radius of the particle, z_i the position of the particle in the vertical direction, and r the radius of the particle. Equation (2) is used to detect collisions that occur, so that there are no collisions between particles, the condition is given $\varphi_{zi} < 0$.

B. Simulation with Fortran

Simulation with Fortran software is divided into several parts including the core program, sub-programs, and several subroutines. This subroutine is used to generate initial position and initial velocity values, define the variables and parameters used, calculate the contact force used on static or dynamic systems, numerical solutions using the gear predictor-corrector method, and the result is a printed image in the form of a postscript file. for each particle movement in a certain time. The results of the images in the postscript file are converted into jpg files, then the final step is to make a movie with Windows Movie Maker software.

The simulation uses a total of 900 particles with various diameter sizes. Particle diameter sizes are generated randomly and then the particles are dropped one by one or at the same h_0 height. The second particle is dropped after the first particle reaches a distance that allows the particles not to collide with each other. If collisions occur between particles, the colliding particles will be knocked off in an unexpected direction or the particles will be reflected up again, causing the desired bumps to not occur. This can be done by adjusting when the collision between the first and second particles occurs, that is, when the first particle has traveled a minimum distance as far as the sum of the radii of the two particles using (1).

The distance traveled by a particle that is dropped freely, is formulated as follows:

$$s = \frac{1}{2}.g.t^2 + v_0.t \tag{3}$$

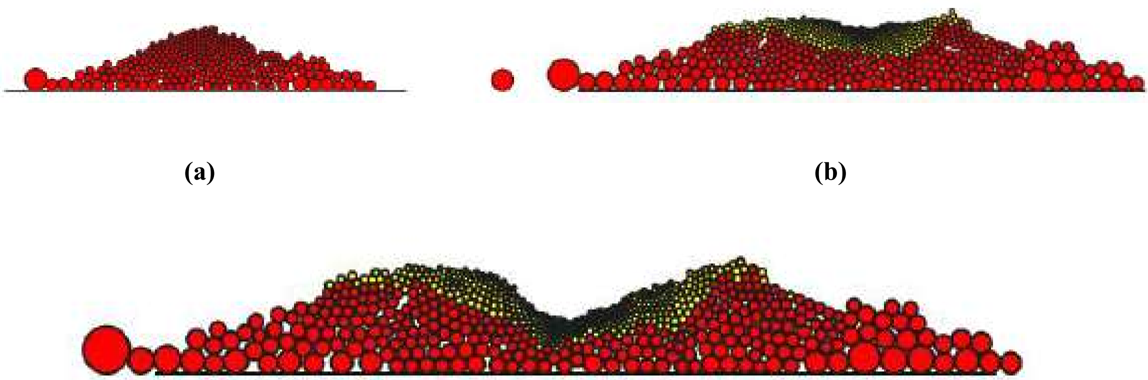
where g is the acceleration due to gravity (9,81 ms^{-2}), t is the travel time, and v_0 is the initial velocity when the particle is dropped. If n is the number of iterations or steps that have been carried out and Δt is the time step or iteration time, then the travel time t is defined by $t = n.\Delta t$. The number of iterations that occur determines when the second particle must be dropped so that it does not hit the first particle where it was dropped. Generating random numbers for particle diameter sizes, the largest particle diameter values are obtained, namely $\varphi = 0.121\, m$, travel time $\Delta t = 10^{-5}\, s$, and initial velocity $v_0 = 0$. The number of iterations n is obtained by inputting these parameters into (3) so that the value $n \approx 15.706$ is obtained so that $n = 15.800$ is selected. If the initial velocity $v_0 \neq 0$ then the result of the n calculation above becomes smaller, so the choice $n = 15.800$ is a safe choice so that the second particle does not hit the first particle where the particles were dropped.

The resulting image is a postscript file for each printed image after 50.000 iterations and produces 730 postscript files from 16.135.700 predetermined steps. These images are compiled into a video with Movie Maker software to determine the movement of the deposited particles as a whole per unit time before the mound is formed until it reaches a stable condition. This condition is referred to as a dynamic condition. Next, the resulting 730 postscript files are made into a movie and presented on https://youtu.be/nQEgizgJFOY. Through the film, you can see the movement of the particles in their dynamic conditions.

C. Equations

Effective conditions can be created by arranging which particles are dropped first so that the mounds that are formed are as maximal as possible in terms of the amount and capacity of the media or space available to accommodate the particles. An effort to see the expected maximum conditions, experiments were carried out by creating conditions where deposition was carried out starting from the largest particle diameter to the smallest diameter (descending) assuming the mass of the particles was the same even though the diameters varied.

Here we present Figure 5 which is the result of deposition of polydisperse particles with descending sequences during static conditions:



(a) **(b)**

(c)

Fig. 5. Stable pile of polydisperse particle with descending order size

Based on the simulation results, the dynamic behavior is that the largest particles that fall first spread to the bottom of the base medium. One-third of the dropped particles accumulate to form triangular particle mounds with irregular surfaces similar to ordinary particle deposition (Figure 5a). The dropping of the particles continues until a number of other particles are getting smaller.

Smaller diameter particles continue to fall right at the center of the mound, until finally the larger particles below bear a much heavier burden because there are far fewer of them. Based on the number, the large diameter particles at the bottom are less than the small diameter particles at the top. Because the gravity acting on the particles at the top is greater than the gravity of the particles at the bottom, the large number of small diameter particles pushes the large particles below. The smaller particles at the top with the greater force succeeded in shifting the large diameter particles to the right and left and then their position was replaced by small particles.

Based on Figure 5b, it can be seen that the particle mound has begun to form a depression in the middle of the mound. The longer the small particles that fall in the middle of the mound the more particles so that the depressions that are formed are also getting steeper. Therefore, after the entire particle is dropped to a static condition, it produces a triangular-like particle mound that has more than one peak, and seems to form two connected mounds (Figure 5c).

III. CONCLUSION

Simulation of deposition of polydisperse particles by ordering the process of falling in descending order produces a mound of particles that resembles a triangle but has two peaks and seems to form two mounds that are connected to each other. The static condition is caused by the dynamic condition of the particle dropping process that occurs. This does not apply if the mass of the particles is different for each different particle size that is dropped.

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