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DEM ANALYSIS OF EFFECT OF THE PARTICLE SIZE DURING THE MATERIAL FLOW IN WEDGE-SHAPED HOPPER

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ABSTRACT

The current analysis was mainly focused to the study of the strained physical effects arising from a decrease of the particles number. The main aspects concerning programming concepts as well as languages having influence on the computer time of simulations is also presented. The limitation in the particles amount was adopted by increasing the particle radii to keep constant the total mass of granular material. In this way, the performed computer simulations of the filling and discharge in three-dimensional hopper using 1980, 10000 and 20400 number of particles were shown that the decrease in particles number with increasing the particle radii produces an artificial friction due to material homogeneity. This is results in the decreased mass fraction and its rate during discharge causing the longest time for the full material discharge; the decreased normal and increased shear pressure of walls.

KEYWORDS

Discrete element method, programming concepts, material heterogeneity, wedge shaped three-dimensional hopper

1. INTRODUCTION

Transportation and handling of granular materials are important components in many industrial processes. Indeed, containers as well as similar storage devices operating within fully automated industrial lines present computer controlled mechatronic systems. Design and monitoring of such systems mainly involve knowledge on granular material behavior under various conditions imposed. Therefore, the computational technologies and virtual models have been recently employed in modeling engineering processes. Engineering characterization of granular material behavior devoted to hopper design is given by Roberts [1].

As a rule, modelling of granular materials has been recently reserved for the continuum mechanics. However, the evaluation of individual particle micro properties of on the dynamical behavior of

granular material as a whole is pursued as highly complicated task for continuum approach. Meanwhile, a unified theory involving evaluation of material micro and macro properties is not established.

Contrary to the continuum-based methods, the discrete concept enables simulation of the dynamical behavior of granular material by direct introspection of physical effects of individual particles on the resulting behavior of static and flowing granular material without any global assumptions. Here, the granular material is modeled as an assembly of particles, while all dynamical parameters (position, velocity, etc.) and inter-particle contact forces are tracked during the simulation. The discrete element method (DEM), based on this concept, has been originally proposed by Cundall and Strack [1].

However, the disadvantages of the DEM technique are basically related to limited computational capabilities caused by a small time step required for time integration equations of motion as well as a limited number of particles involved in simulation. In addition, most of the CPU time is spent on finding the contacts between the particles, which cannot be simply vectorised.

As a rule, straight forward solution of real hopper problems requires a relatively huge number of particles. Due to the presence of diverse scale lengths combined with geometrical complexity of the hopper, typical minimum problem sizes for 3D applications generally range from 1000 to 50000 particles [3]-[7]. 3D DEM simulations have to date been limited to the lower end of this range of complexity and size. It is nevertheless true, that even applying a small amount (~2000) of particles, a sufficiently adequate representation of continuum-based flow parameters was obtained by investigating the granular material flow in hoppers [3], [4], [8].

Even a rapidly increasing computer speed technologies or parallel DEM codes do not enable us resolving numerically the problems with a million p) articles due to extremely long time required for simulation. Therefore, the up-scaling technique may be adopted for the modeling purposes [9]. However, the upscale approach for the modeling of granular material behavior in hoppers has not been found in literature. On the contrary, the simulation time rapidly decreases by limiting number of particles, while the insufficient amount of particles adopted in the model can cause the strained physical effects.

The current analysis was devoted on the study of the effect of particle size in terms of their contribution to the particular bulk material parameters. For this end, the following approach is adopted, particularly; the limitation in the particles amount is accounted for increasing the particle radii to keep constant the total mass of granular material. Accordingly, three samples of granular material having approximately equal masses, but composed by the particles of different size were considered. Particular samples were characterized by 20400, 10000 and 1980 particles. The granular material structure and flow parameters, such as, the system total kinetic energy, the mean coordination number of particle, the discharge mass fraction and its rate as well as hopper wall stresses are studied for characterization of the size effect.

2. MAIN RELATIONS

The granular material is considered as N number of spherical particles with geometric representation of their surfaces and description of physical state. The composition of the media is time-dependent since individual particles undergo variation of their position due to free rigid body motion or due to contact with the neighboring particles or the walls. Newton's second law is applied to each particle i evaluating its translational and rotational motions according to [10]:

$$m_i \frac{d^2 \mathbf{x}_i}{dt^2} = \sum_{j=1, j\neq i}^{N} \mathbf{F}_{ij} + m_i \mathbf{g}\,, \tag{1}$$

$$I_i \frac{d^2 \boldsymbol{\theta}_i}{dt^2} = \sum_{j=1, j\neq i}^{N} \mathbf{d}_{cij} \times \mathbf{F}_{ij}\,, \tag{2}$$

$$\text{where } \mathbf{F}_{ij} = \mathbf{F}^{e}_{n,ij} + \mathbf{F}^{v}_{n,ij} - \mathbf{t}_{ij} \min\left(\left|\mathbf{F}^{st}_{t,ij}\right|, \left|\mathbf{F}^{dyn}_{t,ij}\right|\right), \tag{3}$$

in which $\mathbf{x}_i$, $\boldsymbol{\theta}_i$ are the vectors of the position of the center of gravity and the orientation of the particle, mi is the mass of the particle i ($i = 1, N$), I_i is the inertia moment of the particle, t is the time considered, g is the vector of gravity acceleration, $\mathbf{d}_{cij}$ is the vector specifying a position of the contact point with respect to the centers of the contacting particles [10], $\mathbf{F}^{e}_{n,ij}$ and $\mathbf{F}^{v}_{n,ij}$ are the vectors of elastic and viscous damping force normal to the contact surface [10], $\mathbf{F}^{st}_{t,ij}$ and $\mathbf{F}^{dyn}_{t,ij}$ are the vectors of static and dynamic friction force in tangential direction to the contact surface [10], $\mathbf{t}_{ij}$ is the unit vector of tangential direction originated from the contact tangential velocity of colliding particles i and j [10].

The numerical solutions of differential equations (1-2) for each particle i at the time $t + \Delta t$ (where Δt is the time step) is performed by using 5^{th} – *order Gear's predictor-corrector* [11] scheme.

3. PROGRAMING REALISATION

3.1. Background

To model granular material behavior, two programming concepts based on procedural and object-oriented programming (OOP) approaches may be implemented through different programming languages [12].

Surprisingly, in spite of the problem size, the adoption of the programming concept and languages has a crucial influence on CPU time in DEM simulations [13]. The intense computation nature of the probleme could at times involve simulations running for weeks and thus faster and easily maintainable code is necessary. For this end, three software versions called DEMMAT, based on the above mentioned concept, are described below.

3.2. Run time tests results

The object-oriented programming concept (implemented via C++) was compared with the procedural approach (using FORTRAN 90) in order to test their efficiency [13]. It was compared the CPU needed to model the particle behaviour for their settling on the bottom due to the gravity force, and, later, their compression by moving wall. A comprehensive analysis of these tests was given in [13], [14].

The numerical results obtained in [13] have been shown a significantly better performance of the procedural approach. The code developed in FORTRAN 90 by using the procedural approach was run by about 5-5.5 times faster than the code developed in C++ within the object-oriented approach in the manner de-scribed above. However, these results may be renewed in the light of new advances in language compilers, PC processors.

Thus, the below presented simulation on the particles behaviour in three-dimensional wedge shaped hopper is performed using software DEMMAT [14], developed implementing the procedural concept.

4. SIMULATION AND ANALYSIS

4.1. Simulation setup

Three granular materials, varying from each other by the particle size and its number, were filled into wedge-shaped hopper. The filling is simulated by the sedimentation of particles *en masse* [7]. After achieving a quasi-static state the orifice was opened. A details on the creation of the filling and discharge procedures were given in [7], [8]. The configuration of the hopper is presented as a three-dimensional wedge-shaped wall structure (Figure 1).

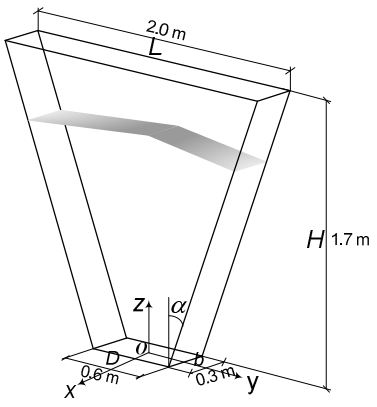

Figure 1 The main hopper geometry

The hopper walls assumed to be rigid representing their as fixed frictional boundaries. Friction and viscous damping coefficients of the walls are assumed to be the same as those used for the particles. The major data on the particles' material is given in **Table 1**.

Table 1. Major data on the particles' material

Quantity	Symbol	Value
Density, kg/m^3	ρ	500
Poisson's ratio	ν	0.30
Elasticity modulus, Pa	E	$0.3 \cdot 10^6$
Shear modulus, Pa	G	$0.11 \cdot 10^6$
Friction coefficient	μ	0.3
Normal viscous damping coefficient, 1/s	γ_n	60.0
Tangential viscous damping coefficient, 1/s	γ_t	10.0

The hopper geometry is defined by the overall height H, the length of the top edge L and the outlet dimension D (Figure 1). The half angle of the hopper is equal to $\alpha = 22^0$. A description of walls as a mathematical model for representation of the boundary conditions is defined by using the rectangular planes of a finite size with their own local coordinate system. The model details were given in **Table 1**.

Thus, three samples of granular material having approximately equal masses, but composed by the particles of different size were considered. Particular samples were characterized by the number of particles, i.e., $N = 20400$, $N = 10000$ and $N = 1980$.

Thus, the aforementioned models were generated by implementing the following approach. In particular, the total mass of particles, mainly influencing wall pressure, and particles volume were held a constant for all models. It was assumed that the total mass of particles is $m_{tot} = 143.57$ kg, corresponding to the total volume of particles $V_{tot} = 0.287$ m^3, for the given particle density.

The granular material composed of poly-dispersed particles was generated by using an uniform distribution. The ratios of the maximal and minimal radii of particles to their mean radius are held the constant for all models. These ratios are simply expressed as follows:

$$k_1 = \frac{R_{max}}{\langle R \rangle}\ ;\ k_2 = \frac{R_{min}}{\langle R \rangle}\ , \tag{4}$$

where R_{min}, R_{max} and $\langle R \rangle$ are the maximal, minimal and mean radii of particles, respectively.

The mean radius of particles is found in terms of the initially assumed total volume of particles using the following relationship

$$\langle R \rangle = \sqrt[3]{\frac{3V_{tot}}{4\pi N}}\ , \tag{5}$$

Finally, the minimal and maximal radii of particles, needed for generation of the particles using the assumed distribution is found from expressions (6) and (7) by multiplying the average radius of particle by k_1 and k_2. The following values of these ratios were assumed: $k_1 = 1.134$, $k_2 = 0.851$. Thereby, the average radii of particles, different for all models, equal to 0.0324 m, 0.0189 m and 0.0149 m for $N = 20400$, $N = 10000$ and $N = 1980$ models of particles, respectively were found. Finally, it should be noted that the generated total mass of particles had a difference from the expected value by about 0.5%.

4.2. Results and analysis

The macroscopic particles structure and flow parameters, such as, the system total kinetic energy, hopper wall reactions and stresses were selected for the sake of adequacies with the main model. A model containing 20400 particles was assumed to be a main indicator in terms of its representation of continuum-based flow parameters due to relatively large number of the particles used. Other models were selected to investigate influence of the particle size and its amount on the material flow parameters.

The structure of granules after filling obtained for three aforementioned models is depicted in **Figure 2**. The particles are colored by using a scalar, with $f_i = \sum_{i \neq j} \left| \mathbf{F}_{ij} \right|$ representing the sum of inter-particle contact forces acting on the particle.

As can be seen in **Figure 2**, the variation of particle contact forces indicates that force transmission within the granular material varies, in particular, at the lower part of the hopper. It can also be

observed, that the amount of particle induces an increase of the local heterogeneity of particle contact force transmission. It can also be demonstrated that there are some particles subjected to much higher forces in the model with 1980 particles as compared to other model. This fact may be partially related to local arching of particles at the lower part of the hopper at the end of filling. In comparison with other models, a much higher particle contact forces are obtained for the model with 1980 particles due to the higher size of particle used producing, in turn, increased gravity force for the given particle.

Consider the total kinetic of the system for the filling process (Figure 3). The total kinetic energy is computed by the summation of the particle energies produced by rotational and translational motions.

Generally, the rapid increase of the total kinetic energy (Figure 3) within 0.5-1 s is explained by the falling of the particles into the hopper with developing vertical velocities with time. A rapid decrease in the total kinetic energy within 1-2.5 s means that most of the particles have dropped on the bottom and cannot essentially change their positions with respect to their neighbors. The increased number of contacts induces the slowdown of particle fluctuations.

As can be seen in Figure 3, the character of variation of the total kinetic energy during the time period 0-3s is almost identical for all models considered. The material models with 10000 and 20400 particles tend to produce the same variation in the total kinetic energy within the entire period of the simulation. Meanwhile, the decrease in the total kinetic energy for the system containing 1980 particles is sufficiently larger in comparison with other models after time instant of 3s, This can be explained as follows, the decrease in the amount of particles (with increasing the particle radii) produces certain heterogeneity of material causing an additional friction effect which, in turn, results in an increased dissipation. It is noticeable, that non-zero shear stresses for frictionless material obtained in [15] have been mainly attributed to a relatively small number of the particles causing certain heterogeneity of material.

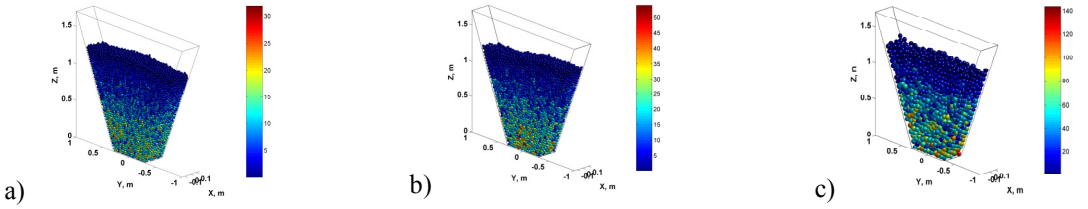

Figure 2 State of granules. Models contain: a) 20400 particles; b) 10000 particles; c) 1980 particles

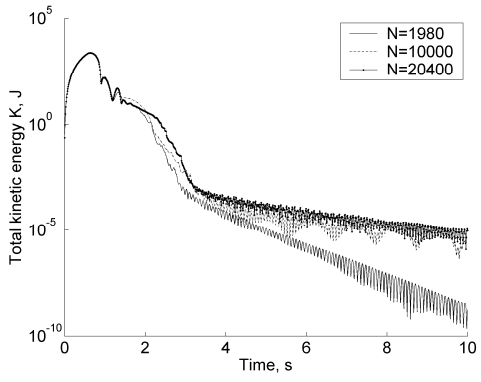

Figure 3 Evolution of the total kinetic energy during filling

Analyse the mass fraction discharged for the material models considered (Figure 4). The mass fraction discharged, $w_f = w_f(t)$, is computed numerically as the ratio of granular material mass discharged to the total mass, while the discharge fraction rate, w, is obtained as the time derivative of w_f.

The graphs shown in Figure 4 demonstrate the different the total time of discharge, $t_f = t\big|_{w_f=1}$ for the material models considered. In particular, the model containing 1980 particles requires the longest time for the material discharge from the hopper, while models with 10000 and 20400 particles show

the shorter discharge times, respectively. The same tendency may be easily proven considering discharge fraction rates depicted in **Figure 5**, where smallest particles have largest discharge fraction rate.

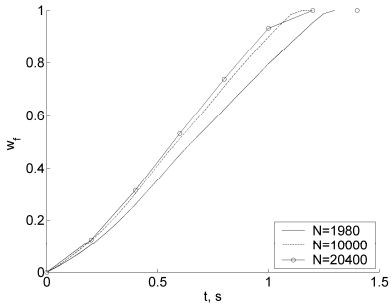

Figure 4 Mass fraction discharged vs time

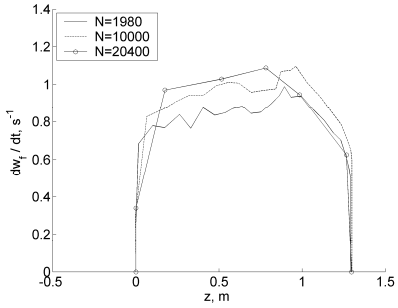

Figure 5 Mass fraction discharged rate vs time

The empirical and simulation evidences that the increasing of particle friction coefficient reduces the fraction and its rate of discharge were demonstrated in [7], [8]. Due to this as well as relying on the results shown in Figure 4, **Figure 5** may be stated that the decrease in the mass fraction discharged and its rate are caused by additional friction induced by the material heterogeneity. This effect relieves with the increasing of the amount of particles in the model.

The effect of the particles amount on wall pressures is also studied. Normal and shear wall pressure components against material depth z^{loc} are depicted in Figure 6.

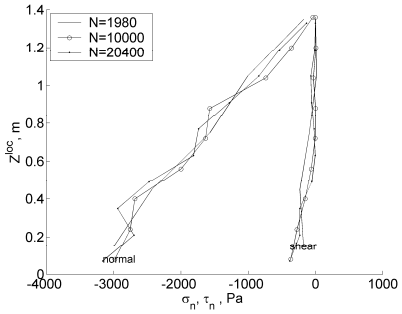

Figure 6 Normal and shear pressures of left wall vs material depth

Theoretically, granular material possessing the friction is able to transmit friction forces, originated from the particle contacts, to the hopper walls. As a result, wall shear pressure grows with the material depth resulting in the non-linear increase in wall normal pressure instead of its linear dependency. In other words, the friction forces developed within the material relieve the normal component of wall pressure, but increase in its shear component. This tendency can be observed in the graphs plotted in Figure 6, where the model with 1980 particles produces lowest normal and highest shear pressure values in comparison with other models. Values of these components for models containing 10000 and 20400 particles are quite close with each other, particularly for shear pressure.

Thus, the obtained decrease of wall normal pressure and increase in its shear component is attributed to the above observed additional friction effect due to material heterogeneity occurred in model with minimal number of the particles. It should be noted that this decrease is quite mild for the current hopper model, but it may be sufficiently larger in a tall hopper.

5. CONCLUDING REMARKS

The current analysis has been mainly focused on the study of the strained physical effects arising from a decrease of the particles number. The main aspects concerning programming concepts ands languages having influence on the computer time of simulations is also presented.

The limitation in the particles amount was adopted by increasing the particle radii to keep constant the

total mass of granular material. In this way, the performed computer simulations of the filling and discharge in three-dimensional hopper using 1980, 10000 and 20400 number of particles have been shown the following: the decrease in particles number with increasing the particle radii produces an artificial friction due to material homogeneity and results in an increased dissipation. Due to this, the model with minimal number of particles produces (in comparison with the large models): a) the decreased mass fraction and its rate during discharge; b) the longest time for the full material discharge; c) the decreased normal and increased shear pressure of walls.

The study performed should be treated as the preliminary investigation indicating that the modification of particle friction coefficient in terms of particle minimal and maximal radii could be developed to obtain the similarity of the models with different amount of particles.

The developed methodology and software could be further extended for non-spherical particles and cohesive materials. Particular application to simulate behavior of cement and asphalt mixtures is also available.

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