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THE EFFECT OF PARTICLE SHAPE ON THE ANGLE OF REPOSE TEST BASED CALIBRATION OF DISCRETE ELEMENT MODELS

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Abstract: Discrete element method (DEM) is a Lagrangian description based numerical technique used for modelling the mechanical behavior of granular materials. For using the DEM model, the micromechanical parameter values used in the governing equations must be determined beforehand. This is the so-called calibration problem. In most of the cases these micromechanical parameters cannot be directly measured, their values must be systematically changed until the modeled macro behavior of the granular assembly will be the same, as the real-life behavior. In this article we propose the simplest possible calibration method, the so-called angle of repose test for application in case of agricultural crop product related problems. We examine the effect of particle shape on the value of angle of repose, ad give statistically acceptable empirical function to describe this dependence mathematically.

Keywords: granular materials, discrete element method, calibration, angle of repose test, asphericity

1. Introduction

The discrete element method was developed for rock mechanics studies in the late 1970s [1]. The method, which was later developed, has now become suitable for modelling almost any problem where granular materials interact with their environment or with each other. The rapid development of informatics enabled us to use DEM for solving mechanical problems arising in agricultural engineering, where most of the products can be modelled as granular assemblies. However, because of the large number of particles and time steps and the various micromechanical parameters which can really increase the computational time, it is still challenging to use this method [2].

2. The discrete element method

For modelling the mechanical behavior of the granular material, we used the academic version of EDEM 2.7 discrete element software. In the discrete element model the simulation evaluates the contact forces according to the “Hertz-Mindlin no slip” contact model: the material and interaction parameters have their effect on the normal- and tangential forces. These forces and moments acting between the interacting soil particles in the form of the following equations [3].

The normal force is

$$F_n = \frac{4}{3} E_0 \delta^{\frac{3}{2}} \sqrt{R_0} - 2\sqrt{\frac{5}{6}} \frac{\ln C_r}{\sqrt{\ln^2 C_r + \pi^2}} \sqrt{2E_0 \sqrt[4]{R_0 \delta}} \sqrt{m_0} v_{\mathrm{nrel}}, \tag{1}$$

where $\frac{1}{E_0} = \frac{1-\nu_1^2}{E_1} + \frac{1-\nu_2^2}{E_2}$ is the equivalent Young modulus of the two interacting soil particles, δ is the overlap between these two soil particles. This normal overlap represents the normal deformation of a particle. The

normal overlap δ between two particles i and j at positions x_i and x_j (where x is the distance measured on the line connecting the centers of the two overlapping particles) with radii R_i and R_j is defined as: $\delta = R_i + R_j - (x_j - x_i)$.
$R_0 = \frac{R_1 R_2}{R_1+R_2}$ is the equivalent radius, $\mathrm{m}_0 = \frac{\mathrm{m}_1\mathrm{m}_2}{\mathrm{m}_1+\mathrm{m}_2}$ is the equivalent mass and v_{nrel} is the normal component of the relative velocity of the soil particles.

The tangential force is

$$F_t = -8G_0\sqrt{R_0\delta}\delta_t - 2\sqrt{\frac{5}{6}}\frac{\ln C_r}{\sqrt{\ln^2 C_r+\pi^2}}\sqrt{2G_0}\sqrt[4]{R_0\delta}\sqrt{m_0}v_{\mathrm{trel}}, \tag{2}$$

where $\frac{1}{G_0} = \frac{2-\nu_1}{G_1} + \frac{2-\nu_2}{G_2}$ is the equivalent shear modulus of the two interacting soil particles, δ_t is the tangential overlap between the two particles and v_{trel} is the tangential component of the relative velocity of the soil particles. The tangential overlap is the tangential displacement of the contact point up to the point at which the contact ends or the particle begins to roll or slip. The tangential overlap represents the tangential deformation of a particle. The tangential force is limited by Coulomb friction $\mu_s F_n$, where μ_s is the coefficient of static friction.

The moment from rolling friction is $M_r = -\mu_r F_N R_i \omega_i$, where R_i is the distance of the contact point from the center of the i-th soil particles and ω_i is the unit angular velocity vector, which is a dimensionless quantity representing only the direction of rotation of the i-th soil particle. μ_r is the coefficient of rolling friction. The tangential force also has moment on the particle: $M_t = F_t R_i$.

During the simulations, the linear- and angular momentum theorem is used to write the equation of motion for all the individual particles resulting multiple number of differential equations to be solved in a sufficiently large number of time steps. The used time step has a great impact on the stability of the numerical model. We selected for the simulation 25% of the Rayleigh-type time step:

$$\delta t = 0{,}25T_R = 0{,}25 \cdot (0.1631\nu + 0{,}8766)^{-1}\pi R\left(\frac{\rho_p}{G_p}\right)^{\frac{1}{2}} \tag{3}$$

It is important to consider that the quality of the obtainable solution could sensitively depend on the value of this time step used during the simulations. The same time step must be used during the calibration process of the discrete element model and during the simulations.

3. Materials and Methods: the angle of repose test

Finding the micromechanical parameters governing the above listed mechanical interactions is not a trivial task [4]. There is no robust method for DEM calibration, results are highly dependent on micromechanical parameters [5]. Because of this the usual way of finding these parameters is based on the simulation of the macromechanical behavior of the particle assembly. The parameters are modified until the micromechanical parameters used are resulting in the same macromechanical behavior in the current model than in the real life. Different techniques are applied for this, for example shear test [6]. [7] was suggested a combined friction model for calibration based on single particle behavior but from the application point of view the easiest solution is the calibration based on angle of repose test (Figure 1.). The most important property of this test, that there is no need for any special apparatus to do it, so it can be done easily and rapidly.
[8] showed how the results of a typical calibration test using a lifting cylinder for the angle of repose (AoR) test are invariant regarding the considered particle size and the dimensions of the test rig, however, the dimensions of the test rig become important for cohesive or elasto-plastic soils according to [9].

Three different techniques for forming conical piles were proposed by [10] using various slumping and pouring procedures to establish a simple calibration method. [11] created a modified draw down test which allows the generation of four experimental reference criteria in one test. Their criteria are the following: AoR test, shear angle test, mass flow rate measurement and the measurement of the discharged mass. We suppose that in our case the angle of repose test is sufficient for doing proper calibration.

Figure 1. Angle of repose test can be done easily and rapidly anywhere

3.1. Discrete element model of the angle of repose test

Material properties which were used in the simulations are shown in Table (1). We used the material properties of corn, because of our further objective is to find the micromechanical properties of corn particles, but this is not the goal of this work. The Poisson's ratios, density of steel, density of concrete and shear modulus of the particles came from literature [12] [13]. The density of particle had to be calculated from the total mass of grains and volume of the cylinder considering the particle shape and porosity of the material assembly. We modified the particle density until the desired bulk density has been reached. The shear modulus values of steel and concrete are the minimal values of the software because in this case the examined material is only the particle so there is minimal effect of these values to the examined results, but computational time is really sensitive to the shear modulus values [12] [13].

Table 1. Material properties used in the DEM simulation

	Material		
	Particle	**Steel**	**Concrete**
Poisson's ratio [-]	0.31	0.3	0.2
Shear modulus [Pa]	$3 \cdot 10^7$	10^6	10^6
Density [kg/m^3]	1180	7500	2400

The interaction properties between the particles and the other materials can be seen in Table (2). The values of coefficient of static friction came from literature [12], the coefficient of restitution and the coefficient of friction values are minimum values, in this case the effect of these values are minimal, but the computational time depends on these variables [14].

Table 2. Interaction properties between materials in DEM simulation

	Interaction		
	Particle - Particle	**Particle - Steel**	**Particle - Concrete**
Coefficient of restitution [-]	0.1	0.1	0.1
Coefficient of static friction [-]	0.2	0.2	0.53
Coefficient of rolling friction [-]	0.01	0.01	0.01

Particles were made from two spherical surfaces, the radius of one sphere was $R = 3.8$ mm. For the examination of the effect of the particle shape in simulations, the distance was varied between the centers of gravity of the two spheres from $d = 0$ mm which is a single sphere to the maximum $d_{max} = 7.6$ mm, in this case these spheres have contact only in one point. Different particle shapes can be seen in Figure 2.a.-c.

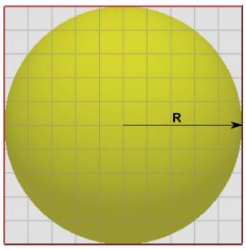

Figure 2.a. Spherical particle with $d = 0$ mm

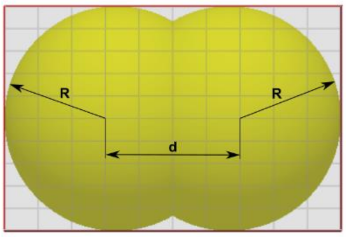

Figure 2.b. Particle with distance d between centers of gravity

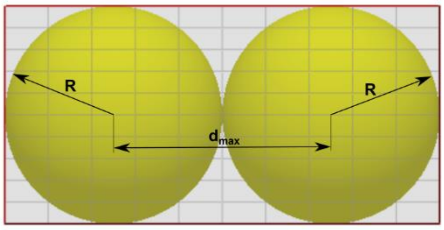

Figure 2.c. Particle with distance d_{max} between centers of gravity

The dimensions of the cylinder geometry can be seen in Figure 3. In simulations a single cylinder with the same $D = 0.2$ m diameter as the cylinder in the corn related measurements was used. The height of the cylinder in the measurements was $h = 0.25$ m and it was fully filled, so the height of the corn pile was the same. Because of settling down of the particles in the simulation, the height of the cylinder must be higher than in reality, it was $h = 0.75$ m. With this h height the h_{pile} was around the original pile height as during measurements. The surface's material was modeled as concrete, and the cylinder as steel.

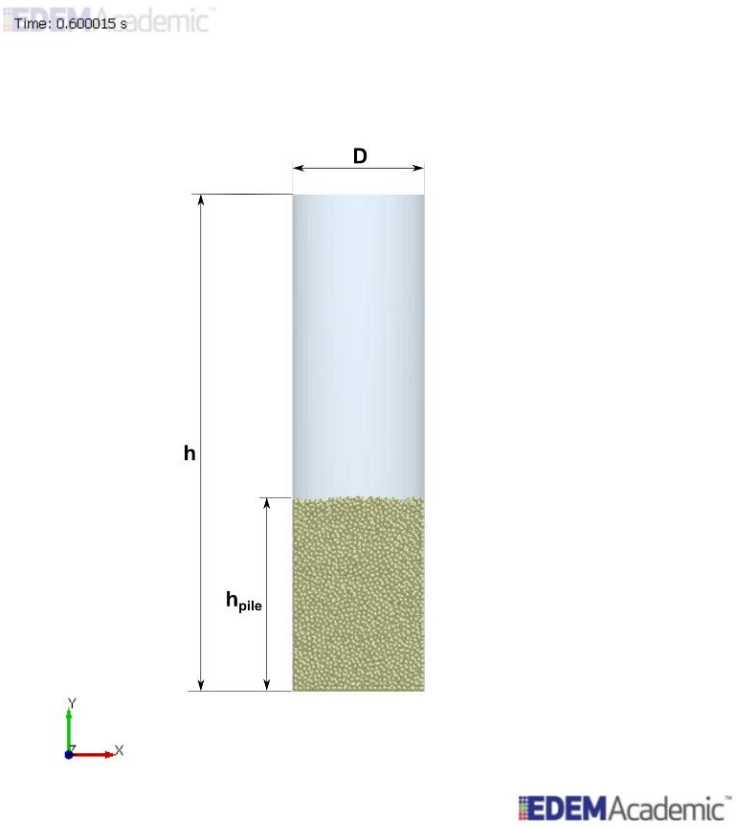

Figure 3. Dimensions of the cylinder in simulations

The number of particles and the mass of one particle was calculated by the software, so the total mass of grains was given. The position of every particle was also calculated in every time step, so when the pile reached the equilibrium state, which was at 0.6 s simulation time, the maximum coordinate y of the pile gave the height of the pile. From the geometrical properties the volume of the cylinder containing the bulk material could be calculated. From the total mass and the volume of the cylinder and the bulk density can be calculated, which is in this case $\rho = 1180 \frac{kg}{m^3}$.

3.2. Data analysis

As it was mentioned above, in simulations the distance d between the centers of gravity of two spheres was varied according to the examination of the effect of particle shape on the angle of repose. Distance d was increased with 1 mm steps from 0 mm to 7 mm, plus $d_{max} = 7.6$ mm case was also applied. 3 repetitions were made in every case.

Particles were settling down in the first 0.6 s, reached the equilibrium state, then the cylinder started moving upwards to direction y with constant velocity $0.11 \frac{m}{s}$. This velocity value was determined from our measurements. The simulation stopped after total time of 2.5 s, when the granular material pile reached the equilibrium state again. After reaching equilibrium state the angle of repose α was calculated from the maximal coordinates x, y and z (Figure 4.), excluding the particles being far away from the pileThe origin of the coordinate system was at the centerpoint of the circle which can be drawn around the pile on concrete floor.

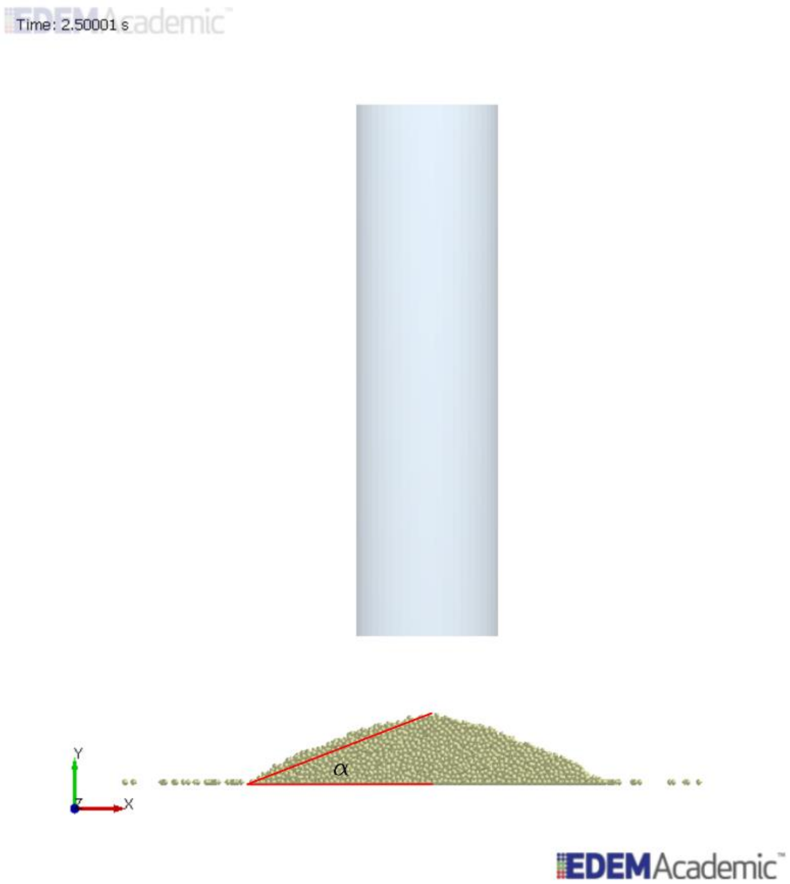

Figure 4. Angle of repose α of the pile

The software calculates the coordinates of centers of gravity of every particle in every time step and α was calculated from the x_{max} and y_{max} coordinates of the pile as the following:

$$\alpha_X = \tan^{-1}\frac{|y_{max}|}{|x_{max}|} \quad (4)$$

Because the pile in equilibrium state is not exactly circular, the angle α was calculated from z_{max} and y_{max} as well, similarly to the calculation above:

$$\alpha_z = \tan^{-1}\frac{|y_{max}|}{|z_{max}|} \quad (5)$$

For further calculations the average value of α_x and α_z was used. Table (3) contains the calculated values with all 3 repetitions.

Table 3. Calculated values of angle of repose with 3 repetitions in every cases

d [mm]	d/dmax [-]	α_X [°]	α_Z [°]	$\alpha_{average}$ [°]
0	0	6.020	6.311	6.165
0	0	6.558	6.370	6.464
0	0	5.917	6.240	6.079
1	0.132	8.299	8.317	8.308
1	0.132	8.467	8.386	8.427
1	0.132	8.103	8.073	8.088
2	0.263	12.385	12.428	12.406
2	0.263	12.258	12.362	12.310
2	0.263	12.148	12.337	12.242
3	0.395	15.359	14.797	15.078
3	0.395	14.999	15.219	15.109
3	0.395	15.111	15.238	15.174
4	0.526	16.592	17.157	16.874
4	0.526	17.666	17.625	17.645
4	0.526	17.474	17.366	17.420
5	0.658	18.765	18.459	18.612
5	0.658	19.272	18.896	19.084
5	0.658	19.429	18.156	18.792
6	0.789	21.255	20.292	20.773
6	0.789	20.079	19.815	19.947
6	0.789	19.612	20.039	19.826
7	0.921	21.795	20.884	21.340
7	0.921	20.695	20.857	20.776
7	0.921	21.394	21.571	21.482
7.6	1.0	21.117	20.886	21.002
7.6	1.0	21.588	22.079	21.833
7.6	1.0	21.571	21.846	21.708

4. Results

In Figure 5, angle of repose α can be seen in function of $\frac{d}{d_{max}}$ which is a dimensionless value varying between 0 and 1.

The diagram shows a trend which has maximum at $\frac{d}{d_{max}} = 1$. A quadratic polynomial function was applied to data points, the equation of the polynomial function is:

$$\alpha = -12.214\left(\frac{d}{d_{max}}\right)^2 + 28.052\left(\frac{d}{d_{max}}\right) + 5.7117 \quad (6)$$

The value of coefficient of determination is $R^2 = 0.9928$ which means a good fitting in this case. According to these data, where the angle of repose at $\frac{d}{d_{max}} = 0$ (this means one sphere) is around 6° and at $\frac{d}{d_{max}} = 1$ is more then 20°, it can be said that the simulation is really sensitive to the shape of particles, that's why using a particle shape which is similar to a real particle shape is important.

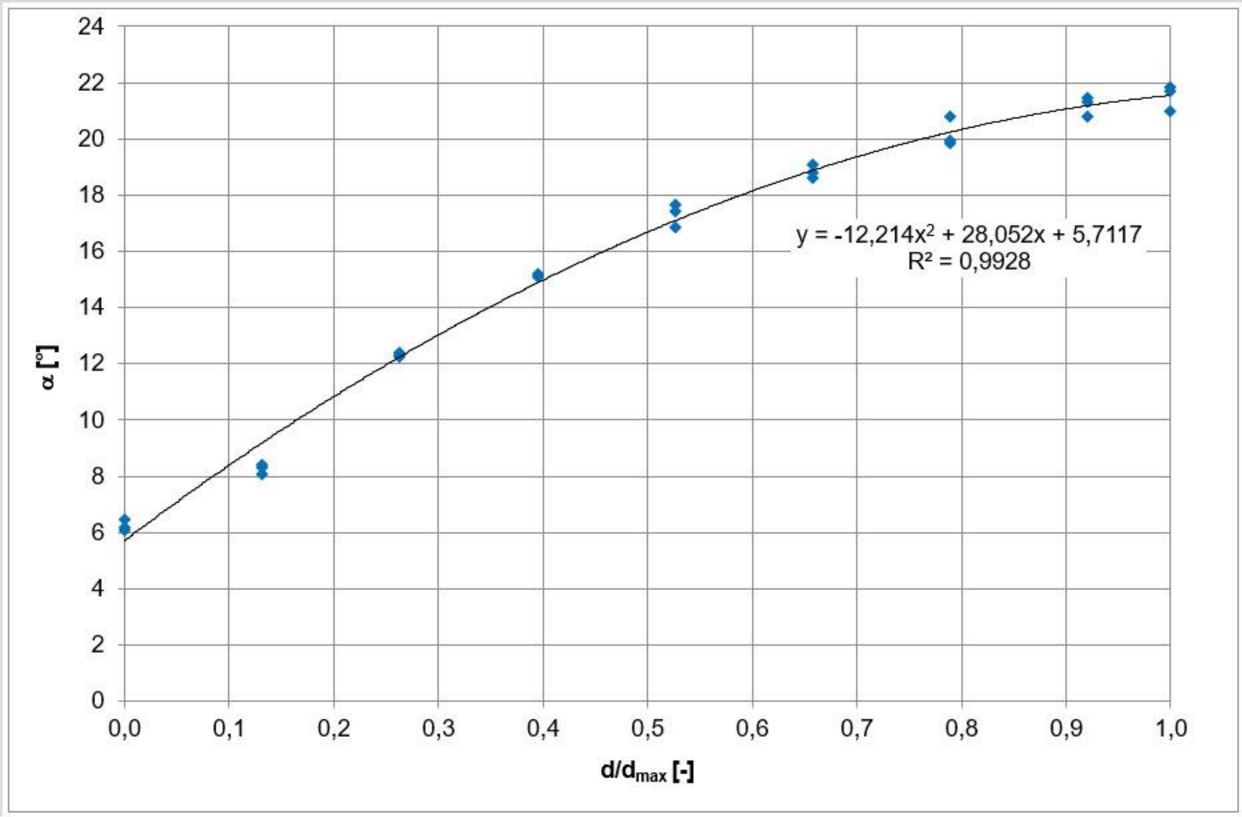

Figure 5. Angle of repose α in function of d/d_{max} dimensionless value

5. Conclusions

The angle of repose measurement is an easy way for finding the data needed to determine the micromechanical parameters of agricultural materials. It is maybe not the best and most accurate measurement, but it can be done anywhere, easily. This makes it the ideal method for calibration measurement. As we have seen in the preceding sections, the discrete element model behavior highly depends on the particle shape. Using the simplest possible non-spherical particle (clump of two spheres) we demonstrated that the angle of repose depends on the asphericity of the particles according to a quadratic function written in the previous section. We suppose that this property is caused by the particles stuck to each other. This result means that during the calibration of agricultural granular material's discrete element models, the geometrical shape of the particles has an important effect on the modelled mechanical behavior.

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