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MATERIAL CHARACTERISATION FOR DISCRETE ELEMENT MODELLING CALIBRATION

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Abstract. The accurate determination of the microparameters needed in a Discrete Element Method (DEM) simulation is essential to obtain reliable results. In this work the DEM model parameters sensitivity in three different laboratory tests (single particle drop test, uniaxial particle compression and rotating drum) are investigated with respect to parameter value changes. The DEM parameters are varied by ± 25% from standard values. Materials used are 3.0 mm soda lime glass spheres and 3.0 mm polyamide spheres. Drop test simulations were sensitive only to change in coefficient of restitution parameter. The single particle compression test indicates that mainly the elasticity parameters influence the numerical response, Young's modulus and Poisson's ratio respectively. The sensitivity analysis indicates that the dynamic angle of repose in simulations depends on static as well as rolling friction coefficients.

1 INTRODUCTION

Developed in the 1970s the discrete element modeling [1] has become a popular simulation tool in the 1990s and its popularity has grown ever since. This rapid increase of DEM popularity is the result of growth of affordable computational power and the available open source and commercial software's.

The calibration of material parameters needed in discrete element method simulations has been a challenge over the last decades [2]. The DEM parameters depend not only on the material's properties but also on the simulation task. Thus, the choice of an adequate calibration test also depends on the dominating granular mechanisms in an industrial process and on the operating conditions. Some of the DEM input parameters, like particle size and shape or particle density, can be directly measured or estimated with a high level of confidence, while parameters like friction coefficients or modulus of elasticity of single particles are often difficult to be measured accurately in experiments, particularly for small particles.

DEM model parameters derived from single particle experiments are rarely sufficient for bulk simulation. In addition, parameters obtained are rarely sufficient for other simulation tasks. Therefore, material parameters have to be calibrated in the process involving gradual change in the DEM input parameters until the simulation results correspond well with the results obtained in physical experiments [3]. The calibration process where only one parameter is modified at a time may be time consuming and lead to macroscopically well correlated results but is obtained with not optimal parameters. Recently, attempts have been made to apply design of experiments (DOE) methods into DEM parameters calibration process [4-6]. The DOE methods help to relate parameters with the simulation output and thus limiting number of required simulations and determining particle properties interactions. The DEM parameter sensitivity investigation indicates the significance of material parameters in simulated processes and, thus, knowing which parameters affect the system of study will help to choose among the possibilities.

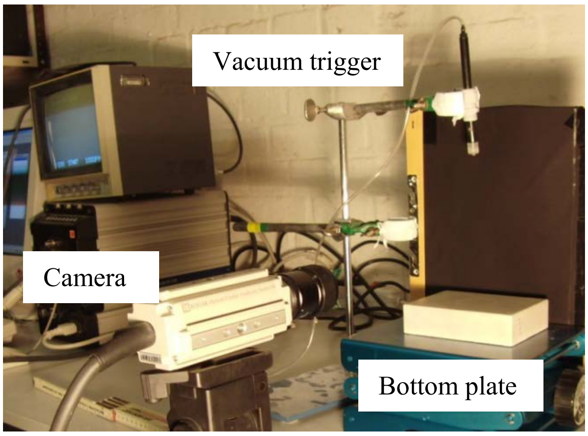
Work presented in this paper focuses on the overview of material properties and a DEM parameters sensitivity analysis to quantify the influence of material properties on simulation results. The DEM parameter values are varied by ± 25%. Three tests are investigated, namely single particle drop test, uniaxial particle compression and rotating drum angle of repose at different rotation velocities.

2 EXPERIMENTAL SETUPS AND SIMULATIONS

A variety of bulk and single particle experiments were performed and compared to its simulations. The experimental setups are presented in Fig. 1. The 3.0 mm soda lime glass spheres were used as a reference material in all experiments and simulations and additionally 3.0 mm polyamide spheres. The DEM material parameters referred here as standard values were obtained in laboratory measurements as explained in [7].

The single particle drop test setup used for spherical particles with diameters larger than 1mm is presented in Fig. 1. Initially the particle is held by a vacuum nozzle 210 mm above the bottom rebound plate. After the vacuum trigger is released, the particle is allowed to fall freely onto a steel, glass or alumina oxide thick-plate. Results of the tests, in which a particle impacts a block made of the same material is referred to as particle wall as well as particle - particle collisions. The mass of the bottom block is many times greater than the particle diameter, so that it creates a stable ground and a reflection of the impact wave does not influence the particle's rebound. Tests were recorded by high speed CCD cameras and the video frames were analyzed to determine the particle's rebound height. For each particle block material combination measurements were repeated until 50 tests suitable for further analysis were recorded. In each of the 50 experiment a new particle was used.

a)



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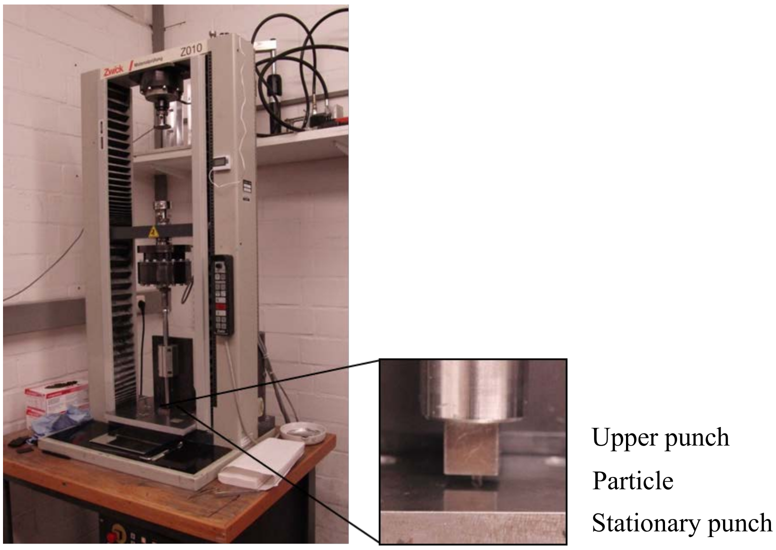

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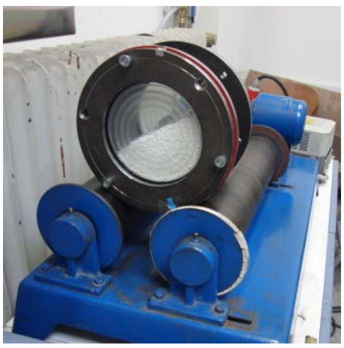

Figure 1: Single particle and bulk experimental setups: a) Single particle drop (homemade); b) uniaxial compression (material testing machine Zwick Z010; Zwick/Roell, Zwick GmbH & Co. KG, Germany); c) rotating drum (homemade).

The single particle compression tests were conducted in a uniaxial material testing machine Zwick Z010 (Zwick/Roell, Zwick GmbH & Co. KG, Germany) as presented at Fig. 1. Experiments were performed for normal compressive loading of one particle from 0 N to a maximum force of 80 N with force resolution of 1 Newton. The sample to be tested was placed onto a lower stationary punch and the upper punch was lowered at a rate of 0.1 mm/min until a first contact is detected. Then the force was reset to zero and the velocity was decreased to 90 µm/min. Once the maximum force was attained the upper punch raises immediately, maintaining the velocity, until 0 N contact force was detected. The experimental setup and a closer look unto a particle placed between the lower and upper punch is given in Fig. 1. The experimental system is computer-controlled with respect to normal forces. The numerical setup where the spherical body to be tested was placed between two plates, resembling a lower stationary and an upper punch, is shown in Fig. 2.

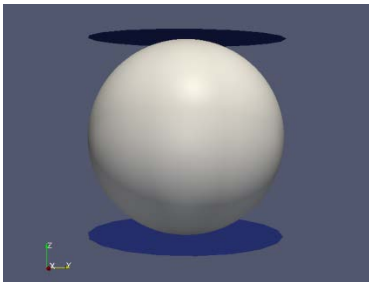

Figure 2: Numerical uniaxial compression setup for a 3.0 mm glass sphere.

A rotating drum of 160 mm in internal diameter and 100 mm long made of steel and glass front and back wall was constructed. The light source pointed at the front wall giving the insight view into formation of material zones of different activity and particle motion (Fig. 1) was used. The drum filled with tested material in 50% was placed on rubber covered metal rods connected to the engine through amplifier allowing to vary the rotation velocities from 0 to over 120 rotations per minute (rpm). Reaching the pre-set rotation velocity, experiments were recorded with a camera levelled at the rotation axis of the drum. Figure 3 shows rotating drum simulation setup.

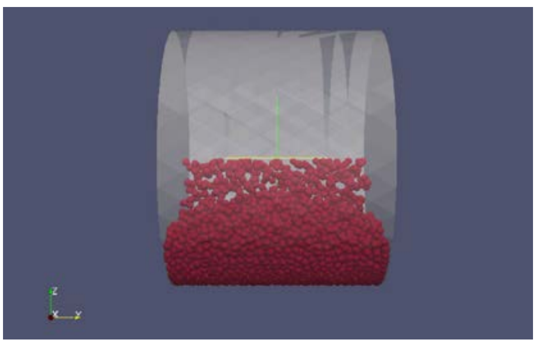

Figure 3: The rotating drum simulation setup.

Table 1 summarizes DEM material parameters used to simulate 3.0 mm glass particles.

Table 1: DEM material parameters: glass 3.0 mm spheres.

Parameter name	Standard value	+25%	- 25%
Young's modulus, Stiffness [MPa]	69000	86250	51750
Poisson's ratio	0.25	0.3125	0.1875
Coefficient of restitution particle - particle	0.95	1*	0.7125
Coefficient of restitution particle – steel wall	0.89	1*	0.675
Coefficient of static friction particle - particle	0.18	0.225	0.135
Coefficient of static friction particle - steel wall	0.3	0.375	0.225
Coefficient of rolling friction particle - particle	0.01	0.0125	0.0075
Coefficient of rolling friction particle – steel wall	0.03	0.0375	0.0225
Particle diameter [mm]	2.98	3.725	2.235
Particle density [kg m^{-3}]	2750	3437.5	2062.5

*maximum possible value equals 1

3 RESULTS

3.1 Single particle drop simulations – coefficient of restitution

The single particle drop experiment of the soda lime 3.0 mm glass sphere on glass plate resulted in coefficient of restitution calibrated to 0.95 and 0.89 between glass particles and steel bottom block. The 3.0 mm polyamide spheres were dropped onto glass and steel bottom plates resulting in the calibrated coefficients of restitution of 0.85 and 0.9 respectively.

The rebound height was expected to be strongly related with material elastic properties. The shear modulus, Poisson’s ratio and material density were varied ± 25% and ± 50%, however no significant nor consistent change in rebound height was observed.

The coefficient of restitution (COR) was tested at 75 % of the standard value and equal to 1 (since this is the maximum possible value). A 25 % decrease of COR in glass - glass collision resulted in the rebound height of just under 100 mm which is 47 % of the drop height. Similar results were observed for other materials and bottom plates. With COR parameter set to 1, rebound heights were moderately lower than drop height for all materials tested.

3.2 Single particle compression test – modulus of elasticity

The impact of the variation of the modulus of elasticity on particle deformation in the single particle compression simulations is presented in Fig. 4. A 25 % increase of modulus of elasticity results in 6 % lower displacement, whereas a decrease of modulus of elasticity increases the displacement by 10 %. The same response was observed when changing the particle diameter: with an increase in diameter the particle was further compressed, while a smaller particle diameter resulted into a lower displacement. A change of 1.5 % displacement was observed for a 25 % decrease and an increase of Poisson’s ratio value. Single particle compression simulations were not sensitive to changes of particle density, particle/particle and particle/wall friction coefficients. An increase of particle wall restitution coefficient results in a small change in forces acting at the wall during compression.

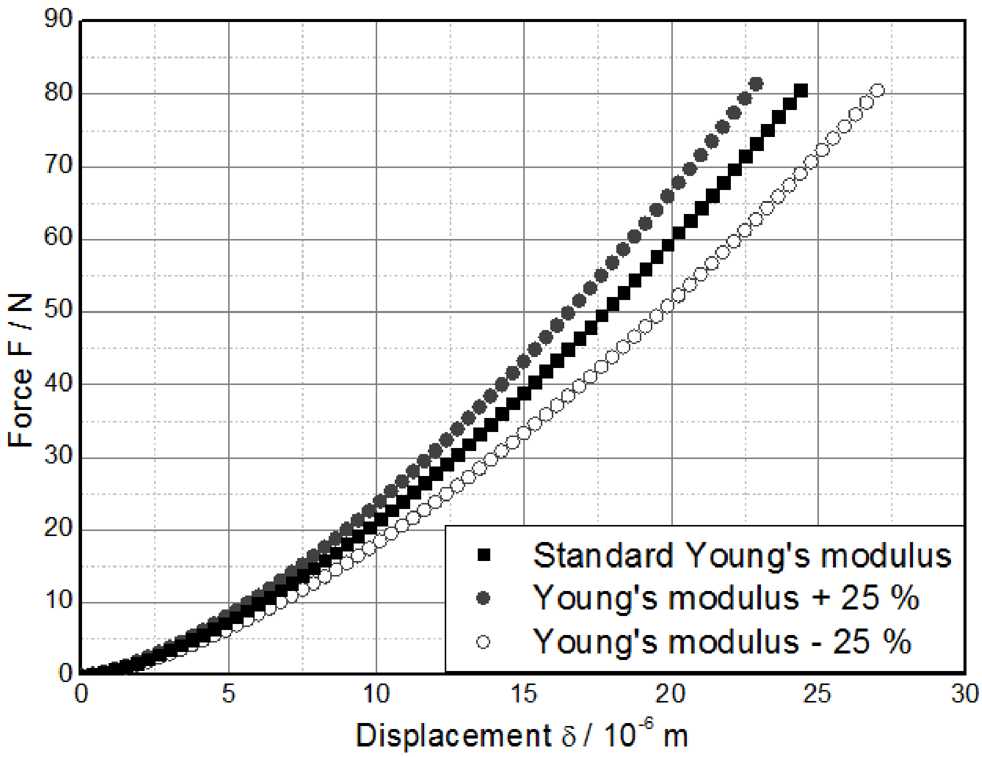

Figure 4: Influence of Young's Modulus on single particle compression simulation results, glass 3.0 mm.

3.3 Pile formation and rotating drum simulations – coefficients of friction

In the rotating drum simulations, the interparticle friction coefficients determined in pile formation simulations were used, whereas friction coefficients between drum wall and particles were based on the wall shear results. The particle - glass wall rolling friction coefficient was set to 0.01 and the particle - steel wall rolling friction to 0.02. The particle – glass wall sliding friction value was set as a 70 % of particle - steel wall sliding friction value, based on the relation observed in shear tests.

For the purpose of this research two rotating velocities were tested: 1 and 30 rpm. At rotation velocity of 1 rpm observed angles of repose were comparable to pile formation results. The angle of repose (AoR) measured for 3.0 mm glass spheres simulation using standard parameters at 1 rpm was 24.1°. Variation of shear modulus and Poisson's ratio parameters had no visible impact on the AoR. Variation of density and interparticle and particle walls coefficients of restitution values resulted in AoR value change of less than 0.5°. Up to 1° of angle of material inclination change was observed while varying the static friction coefficients.

Additionally, polyamide 3.0 mm spheres and 3.0 mm glass spheres were tested in the rotating drum simulations at 30 rpm. Table 2 summarizes measured angles of repose. The angles of repose measured for standard set of polyamide parameters was 43.0°. Very little or no difference was observed when increasing the values of shear modulus and material density and decreasing the Poisson's ratio, but one degree increase was observed when increasing Poisson's ratio and one degree decrease when lowering values of shear modulus and density. The 25 % decrease of COR values resulted in nearly 1° decrease in material inclination angle. Increase of COR value to 1 had little influence.

Angle of material inclination was most sensitive to changes in static friction value. A decrease of 25 % of the interparticle static friction resulted in angle of repose of 40.2°, 42.3° when particle steel drum wall friction was lowered and 42.5° when particle glass drum side wall friction was 25 % lower. Angles of repose of 45.3°, 51.9° and 45.0° were measured when interparticle, particle steel wall and particle glass wall static friction coefficients values were 25 % higher than the standard values. This was in agreement with another sensitivity analysis, conducted with an 81 mm diameter drum of comparable length, but with a filling degree of 25 vol-% and 2 mm spherical particles. In this analysis static friction values were changed by 50 %. Other coefficients were similar, but not equal, except for the Young's modulus, being scaled to 2.5 MPa for calculation time acceleration, not necessarily representing a realistic material value. Nonetheless, this numerical experiment produced the similar result of static friction being the most influential parameter in determining the dynamic angle of repose. Changes in angle of repose were 2° when decreasing these friction coefficients by 50 % and 4° by increasing them.

Table 2: Polyamide 3.0 mm angle of repose measurements, drum 160 x 100 mm, 30rpm.

Parameter name	**Sensitivity analysis output [°]**		
	- 25%	**standard**	**+ 25%**
Young's modulus, Stiffness	42.1	43.0	42.9
Poisson's ratio	43.1	43.0	43.8
Coefficient of restitution particle - particle	42.2	43.0	43.1
Coefficient of static friction particle - particle	40.2	43.0	45.3
Coefficient of static friction particle – wall, steel	42.3	43.0	51.9
Coefficient of static friction particle – wall, glass	42.5	43.0	45.0
Particle density	42.3	43.0	43.1

The 25 % variation of standard values of rolling friction of 0.01, due to a low change in the value, has no visible effect on measured angle of repose. To verify the importance of rolling friction coefficient, parameter value was set to 0.05, resulting in AoR of 46° and 45° for interparticle and particle wall parameters respectively, and 0.1, resulting in AoR of 55° and 52° for interparticle and particle wall parameters. The importance of the rolling friction coefficient was also verified in the 81 mm diameter drum: a 2 to 3° change in AoR was observed for 50 % variation of rolling friction around the value of 0.05 for both particle-particle and particle-wall interactions.

Similar observations are reported for 3.0 mm glass spheres.

3.4 Calibration of DEM parameters

Given a certain system of study and when the DEM parameters that most influence this system are known, the sensitivity analysis of the standard experiments shown before will help to design a procedure to calibrate the DEM parameters needed.

Usually more than one parameter has to be measured at the same time. A very common case for this approach is the calibration of both coefficients of friction. However, as already shown by Wensrich & Katterfeld (2012) [8], angle of repose, for example, can be obtained through many combinations of the friction coefficients. That means that more than one experiment is needed [9].

4 CONCLUSIONS

- The DEM simulations of single particle drop, uniaxial compression test and rotating drum were conducted. DEM parameters sensitivity was investigated.
- Modulus of elasticity has a significant influence on force displacement relation in single particle compression simulations. A small change on particle deformation is observed for variation of Poisson's ratio and coefficient of restitution parameters.
- Single particle drop simulations were sensitive to variation of coefficient of restitution, and not sensitive to change in shear modulus, Poisson ratio and material density.
- Both, interparticle and particle wall static friction coefficients are found to be the crucial parameters governing the material behavior in rotating drum simulations. The rolling friction coefficients has lower impact on the measured angles of repose due to an order of magnitude lower value compared to static friction values.
- Sensitivity studies of DEM parameters in given systems of calibration experiments may be an aid in the calibration of these parameters. DEM parameters can then be calibrated by comparing the macroscopic responses of standard experiments of bulk materials and its simulations.

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