EXPERIMENTAL WORKS FOR VALIDATING A DISCRETE ELEMENT SOFTWARE

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ABSTRACT

The current paper describes the procedure of validating a discrete element software through numerical and experimental models. The comparative models show the behavior of a granular material subjected to punching by a rigid die. In the experimental works, the granular material was created using quasi-spherical and -cubical glass objects, in different combinations, punched by a wooden plate at constant rate. The tests were conducted using typical geotechnical laboratory equipment, with minimum investment in the physical model. The numerical models were created using both the original software and a benchmark program, well established for discrete element modeling (PFC3D). It is shown that finding the necessary input parameters for the numerical models depends on various factors, such as particle material, shape and size, as well as the used modeling software. Some typical geotechnical tests were performed, but the results show they are inadequate for this type of material.

Finally, 19 models were created using the created software, with various setups, and 1 (one) benchmark model using PFC3D. The results display good qualitative data, compared to the physical models, easily shown by the failure mechanism of the material. However, the created software lacks the precision of quantitative results, as opposed to the benchmark software, which is in good agreement with the data obtained by physical tests. This could be due to the way of loading in the proposed software, which uses imposed load and measured displacement, instead of imposed displacement and measured load employed in physical and PFC3D models. In conclusion, the tests show good perspectives for the created software, which is still in the early stages of development.

Keywords: discrete element method, experimental works, numerical modeling

INTRODUCTION

Geotechnical and foundation engineering are fields that require understanding the behaviour of various materials, ranging from steel and concrete, which have a continuous and isotropic character and are created in controlled environment, to soil, which has a rather discrete nature and varies in properties from one site to another. Although numerical models used in practice generally consider the soil to be a continuous and homogenous medium, assumption on which most of the theory describing the behaviour of soils is based on, the true character of the material is actually discrete, in which the interactions between individual particles govern the overall behaviour. Since the introduction of the Discrete Element Method (DEM) by Cundall and Strack [1], which is a discontinuous approach of numerical modelling granular assemblies, many advancements have been made, and several efforts were taken towards applying this approach to better understand the mechanical behaviour of soils. The method focuses on the properties of individual elements from which the material is composed, and allows the study of the continuum even after the failure occurs within, which cannot be done using continuous modelling techniques.

Several DEM codes have already been created, some of them open-source, like LIGGGHTS [2] or YADE [3], or the more established commercial codes PFC3D [4] and EDEM [5], and many others are in development, since the implementation of the algorithms become easier and faster with the upcoming technology. The discrete element software created by the authors [6] has the advantage of adding a simple interface to the program, making it easier for users to create the models, without requiring programming knowledge.

When validating a DEM model, various researchers have employed simple physical tests that can be reproduced numerically (e.g. sand-pile test used by Johnstone [7]) or even classical geotechnical tests, such as the direct shear test, reported by O'Sullivan et al. [8] or Keppler and Csatar [9]. Based on reported experience, the procedure used in this project was focused on the behaviour of a continuous footing foundation model which was simulated both physically and numerically, in a plane-strain approach. A similar set of trials was conducted by Johnstone [7] and has proven to be a good benchmark for DEM validation.

PHYSICAL MODEL

The model was constructed in a glass container, which was filled with two types of glass particles of quasi-spherical (with 6.0mm diameter) and quasi-cubical shapes (with 4.0 mm sides) (fig. 1). Model geometry (fig. 2 left) and the employed materials were chosen so that a plane strain state can be simulated, easy to reproduce numerically. Since the particles used for material modelling was not specially designed for these tests, they have hollow cross-sections, which induces significant inner porosity. However, since water was not modelled, the only influence of this particle porosity is on the particle density, which can be determined with acceptable accuracy, to be reproduced in the numerical models.

Fig. 1: Particles used to as granular material: quasi-spheres (left); quasi-cubes (right)

The tests were performed using a standard triaxial compression frame used for geotechnical purposes (fig. 2 right). The apparatus has a mobile base which can displace on vertical direction at a constant imposed rate. After filling the container with particles, placed in layers based on colour and shape, for better visualisation of the results, the model was rested on the base of the device, while a rigid die was placed on the top of the granular material. A fixed proving ring was used to measure the vertical force produced by the loading die on the granular material.

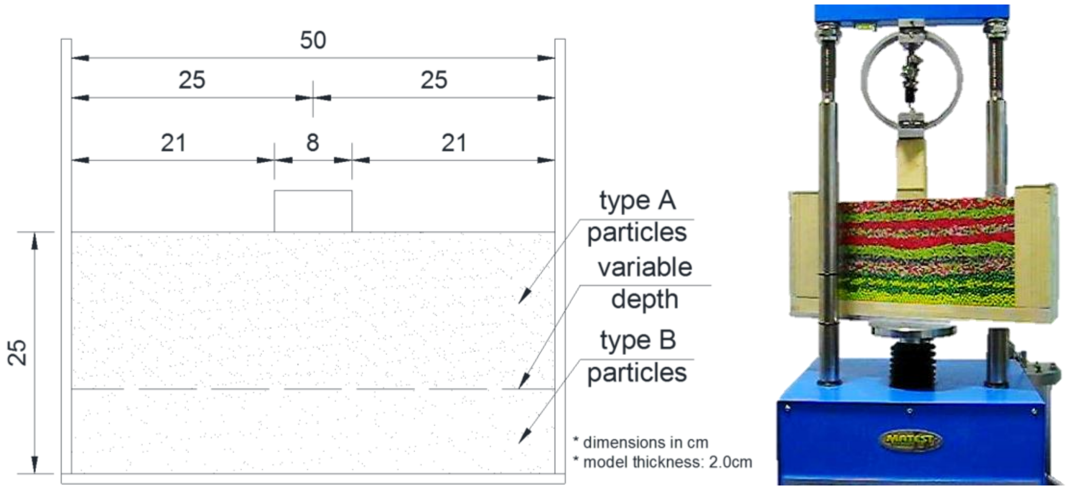

Fig. 2: Model geometry (left) and experimental setup prior testing (right)

The experimental works were conducted by displacing the base of the apparatus vertically, towards compressing the model, at a constant rate, on a maximum distance of 50mm. The setups were based on two structural and three mechanical configurations and, mainly: • cubes (a) or spheres (b) at the upper part of the model (approximately 2/3 of the volume); • displacement rates of (i) 2.5mm/min, (ii) 5.0mm/min and (iii) 6.0mm/min. By recording the normal force measured with the proving ring at various times, load-displacement diagrams were obtained, displayed in fig. 3. More qualitative results are shown in the Results and Discussion section, where they are compared with numerically obtained data and discussed.

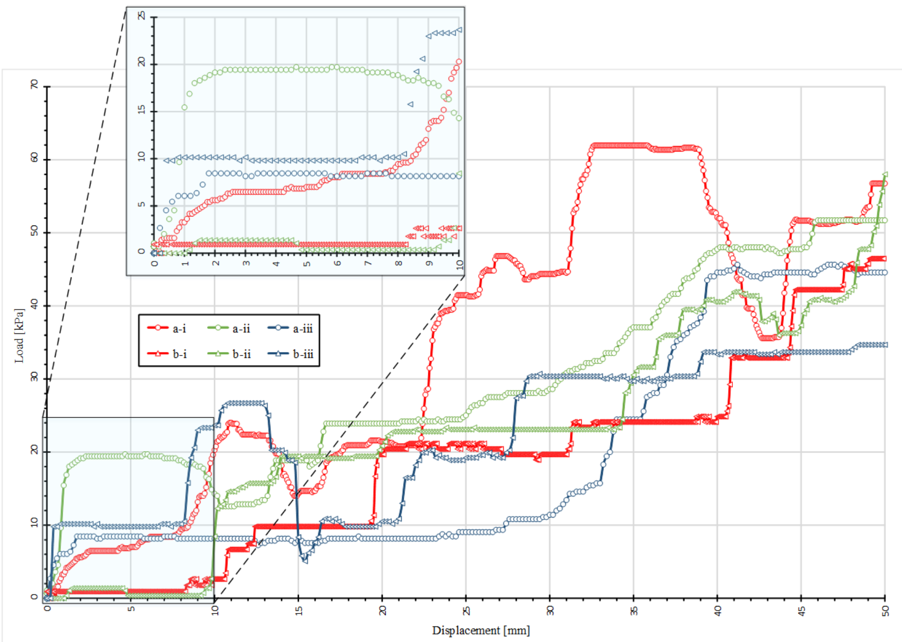

Fig. 3: Load-displacement diagrams obtained for the performed tests

NUMERICAL MODELS

The numerical models were created using both the proposed software [6] and PFC3D [4], which is regarded as one of the leading codes in the field. Depending on the employed program, various parameters are needed to define the behaviour of the material. Using DEM, both physical and micromechanical characterisation of the particles is required in order to accurately describe the material. Unlike FEM modelling, where the material is continuous and global parameters are employed both for physical and mechanical description (e.g. bulk density, porosity, global strength parameters) DEM models require a different approach, by which the individual parameters of the particles are defined in such a way that the overall behaviour of the material is replicated. Since micromechanical parameters required in DEM simulations (i.e. spring stiffness, coefficient of static/dynamic friction and coefficient of restitution) are not always directly measured through laboratory tests, some efforts were made to determine these parameters by tests easy to reproduce numerically and the selected values were chosen by attempting to match the physical results through numerical simulations.

Material parameters assessment

The density of the particles was determined through a series of 20 direct measurements of sets of 10 spheres and 20 cubes respectively, resulting in densities of 2.58g/cm^3 for spheres and 1.33g/cm^3 for cubes. These values correspond to the assumption that the particles have no inner voids. Further on, the inter-particle porosities of compacted material were found by filling a known volume with particles and using a relation between indices:

$$\rho_d = \rho_s\left(1-\frac{n}{100}\right), \text{ thus } n = \left(1-\frac{\rho_d}{\rho_s}\right)100 = \left(1-\frac{m_d}{\rho_s V}\right)100$$

where ρ_d is the dry density of the material, ρ_s is the particle density, m_d is the total dry mass of the material and V is its volume. Thus, the obtained porosities, n, are 45% for spheres and 1% for cubes. Although, according to Keppler's conjecture [10], the minimum theoretical porosity of a volume filled with equal spheres is 26%, numerical tests ran by Benabbou et al. [11] show that the minimum porosity that can be obtained is around 36%. Even with spheres of various diameters, which are able to fill the space more tightly, research by Ferrez [12] or Jodrey and Tory [13,14] suggested that minimum porosities obtained numerically vary between 31% and 47%.

The mechanical parameters needed for DEM simulations are required to characterize the contact behaviour between two particles, known as micromechanical parameters. As opposed to the global macromechanical characterization of the material using continuous models, where typical geotechnical tests are employed (e.g. shearing or compressibility), a different approach is required for DEM simulations. Based on previous research, a set of hopper tests were performed, for measuring the angle of repose of the pile made of granular material.

The material was slowly dropped on a glass bed using a hopper (fig. 4) and the results were digitally processed (e.g. fig. 5 left) so the average angles of repose were obtained for each particle shape, i.e. 20^o for spheres and 27^o for cubes. Although the particles are made of the same material, the smaller angle of repose for spheres can be explained by their smaller resistance to rolling which leads to a wider arrangement of the particles.

Fig. 4: Typical sand-pile test result using cubes: angle view (left); side view (right)

Then, numerical DEM simulations were conducted using the 3D hopper method described in a previous research [15] and a set of 200 results were obtained for each particle shape, which show the variation of the angle of repose with the input contact friction angle (fig. 5 right).

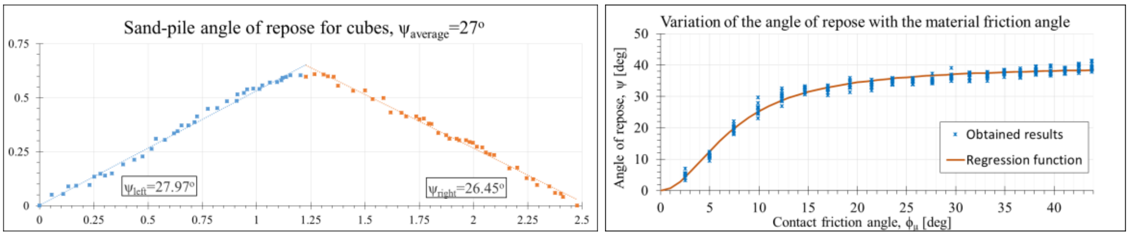

Fig. 5: Processing of the sand-pile physical tests (left); calibration of the contact friction angle using 3D hopper numerical simulation (right)

Although the sand-pile test was widely used in previous projects and has shown good results, e.g. Johnstone [7], it has been reported that various DEM parameters combinations may yield the same macroscopic result, so another type of test was conducted, in which a glass inclined plane was used to determine the inter-particle friction angle of the particles. Only cubes were used for these tests, since their failure on the inclined plane would only be produced by sliding and not rolling. Finally, a 28^{o} friction angle was obtained, which was in good agreement with the angle of repose.

Furthermore, oedometric compressibility and direct shearing tests were used to determine the stiffness of the material and their macromechanical response when sheared. The compressibility tests were conducted up to loads of 1000kPa, and with 3 stages of loading and unloading, and the results showed a stiffness of about 25000kPa on the first loading cycle, between 12.5kPa and 25kPa, and 80000kPa for the reloading cycles, between the same load increments. The sear tests however, have shown no concludent results, since the low resistance of the particle material lead to significant local crushing which renders the results unusable for this type of material.

Numerical simulations

Using the obtained test data, the numerical models were created in the proposed software. The granular material was constructed using the same shapes and sizes as the physical particles, by filling approximately 1/3 of the volume with one type of particles and completing the rest of the volume with the other set. The simulations were based on a modelling plan of 19 tests, with various parameters, for a better understanding of the sensitivity of different parameters. The loads were applied incrementally, and each step was maintained until settlement variation became small enough to be neglected. Since volume filling was performed using a sedimentation algorithm, a set of initial material properties were used to obtain various porosities of the materials, while the friction angle has been changed after the sedimentation, prior to the loading stage. Fig. 6 shows the initial state of the model prior to running the simulation.

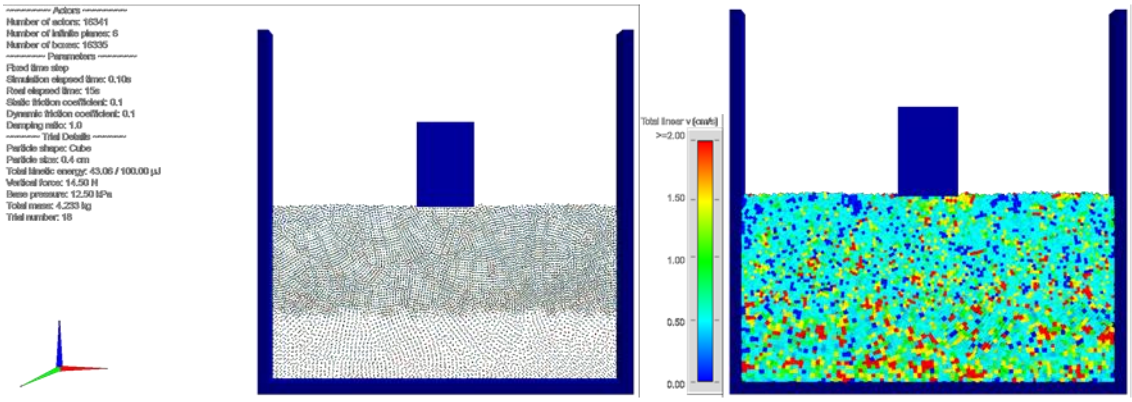

Fig. 6: Typical setup after the sedimentation process, prior to loading: particle centres are shown on the left and real shapes on the right

The benchmark model was created using PFC3D, by employing only spherical particles. Linear spring with friction contact model was used to handle particle contact, where the necessary parameters are contact spring stiffness and friction coefficient. Although compressibility tests were performed for the material, using the obtained values yielded unreliable results. Therefore, various properties were used in an iterative process, based on the obtained porosity of the material, and 10kN/m contact stiffness with 0.5 friction coefficient were selected as the suitable parameters.

Finally, after filling the volume with particles by using a similar sedimentation algorithm as the one used in the other models, the footing was creating using rigid walls and a constant displacement rate was applied to the footing, while results were recorded.

RESULTS AND DISCUSSION

This section shows some of the results obtained physically and numerically, in hopes of showing the similarities and differences between them. Fig. 7 represents the state of the experimental model in which the failure mode can be observed and the area of influence of the die within the material can be seen to spread down to about half of the material depth. Although variations in the 6 experimental setups were made based on particle deployment and loading rate, the results did not show significant differences between the tests.

In fig. 8, the result of the PFC model is shown in a similar manner, and it can be noticed that the material failure mode and area of influence are in good agreement with the experimental works. Displacement vectors of the particles are presented in fig. 9 for the PFC model, while fig. 10 shows the same type of data, obtained through one of the simulations ran in the proposed software. The results in fig. 10 correspond to a model created using cubes at the base and spheres in the upper part, with a micromechanical friction angle of 28^o.

The observed qualitative behaviour of the models are in good agreement and moreover, the load-settlement diagram obtained in the PFC simulation is similar to the results of the physical tests. However, the loads obtained in the proposed software do not correlate well with the measured data. This may be due to the loading approach used, which was done with imposed load and measured settlement. For testing this assumption, an imposed displacement method should be used in the simulations, but this would greatly influence the required computation time.

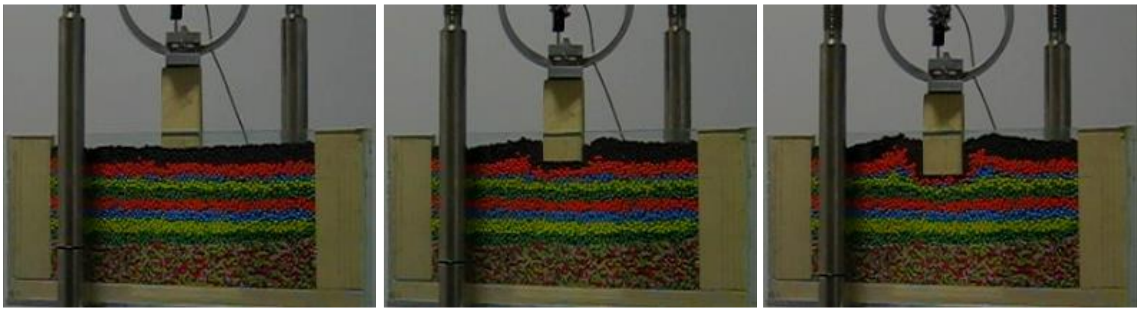

Fig. 7: Physical model state at different stages: initial stage (left); mid-stage (middle); final stage (right)

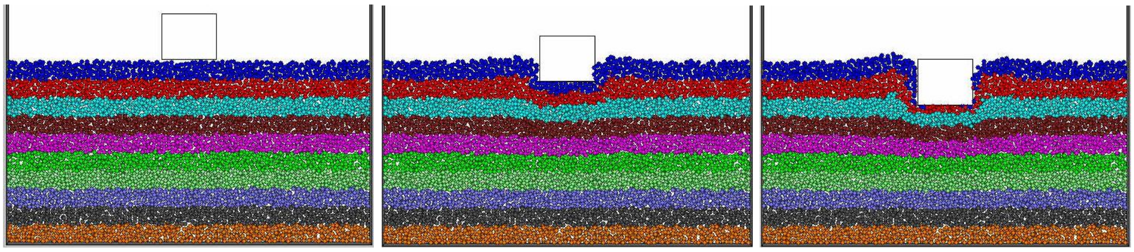

Fig. 8: PFC model state at different stages: initial stage (left); mid-stage (middle); final stage (right)

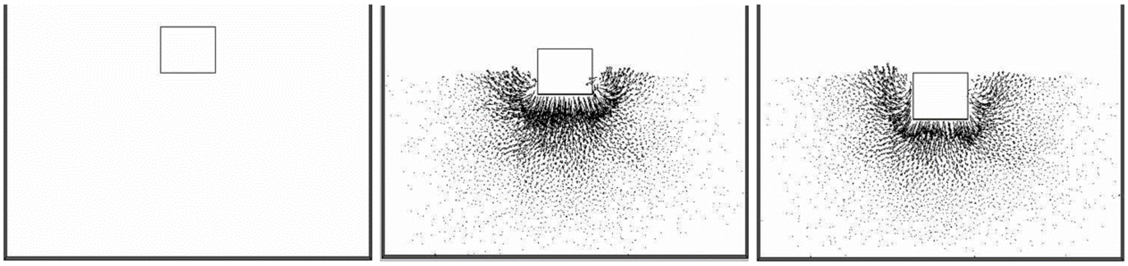

Fig. 9: PFC model displacement vectors at different stages: initial stage (left); mid-stage (middle); final stage (right)

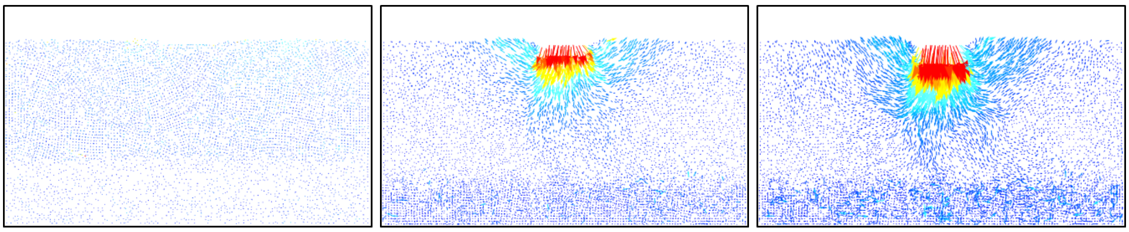

Fig. 10: Proposed software displacement vectors at different stages: initial stage (left); mid-stage (middle); final stage (right)

CONCLUSIONS

The paper has shown a simple way of testing the quality of a DEM software, employing physical models using common geotechnical laboratory equipment. It can be noticed that parameter assessment is probably the most demanding task, since there are no standard procedures and they require a micro-mechanical parameter tweaking for reproducing macromechanical behaviour. However, some simple approaches may be employed, as the hopper test, to easily determine the friction coefficient of the material, while other tests may have limitations depending on the type of material used or the shape of the particles. The obtained results using the proposed software are in good qualitative agreement with the physical data and the benchmark software, however, some improvements are still needed for better quantitative output.

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