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Calibration of the discrete element method and the effect of particle shape

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ABSTRACT

The discrete element method (DEM) is used across a wide range of applications. However, accurate predictions can only be made if the input parameters are carefully selected. In this paper a calibration process is proposed to calibrate the parameter values for crushed rock particles up to 40 mm in size. A large shear box with a diameter of 590 mm was designed and built for this purpose. Confined compression tests were used to determine the particle stiffness and direct shear tests to determine the particle–particle friction coefficient. Two methods were used to create the clump particles: a manual process and an optimised process to create clumps comprising of 2, 4 or 8 spheres. The clump types were individually calibrated to obtain a unique set of parameter values for each. The angle of repose is often used for the calibration of the particle–particle friction coefficient and was included in the calibration process for comparison with the direct shear test results. The calibration process was validated by modelling anchor pull-out tests and hopper discharge using the different clump types. The results showed that care should be taken when the angle of repose is used to calibrate the particle–particle friction coefficient. It can result in a friction value which is too low for use in other applications, although the angle of repose is accurately predicted.

1. Introduction

The discrete element method (DEM) has become the method of choice for modellers and engineers to validate and optimise the design of bulk material handling systems [1–3]. It is estimated that up to 40% of the capacity of industrial plants is wasted because of bulk handling problems [4]. DEM is used over a wide range of applications which include mining [5–6], post-harvest [7], soil-tool interaction [8–14], mixing and milling [15–17] and geotechnical applications [18–19] amongst others. The focus of this paper is on loose granular materials and not on bonded assemblies [20].

Before any DEM modelling can be attempted with confidence, an accurate set of material input parameter values is needed. Therefore, robust calibration procedures are needed that are efficient from both an experimental and numerical point of view.

We distinguish between the material macro properties and the DEM micro parameters. Material macro properties are bulk properties that can be measured and include, for example, resistance to penetration, the angle of repose, the bulk density, the internal friction angle and the bulk stiffness. The micro parameters on the other hand are the parameters used by the specific discrete element method to model the material and include, for example, the particle stiffness, the particle–particle friction coefficient and the particle density. In the literature, micro parameters are often not measured and the values are assumed without justification [8]. How the parameter values were obtained is often not mentioned and whether they were measured or calibrated is not clear. Together with this, the final simulation is often not validated [21].

The particle size and shape distributions are also considered to be input parameters. In DEM codes, spherical particles are usually preferred due to the efficiency of contact detection. However, when using spherical particles, the bulk friction of the assembly is usually too low when compared to real granular material like crushed rock. Two methods to increase the bulk friction exist to be implemented separately or in combination. The one method is to include contact rolling resistance and the other is to make use of non-spherical particles. Examples of non-spherical particles include ellipsoids, super-quadrics, polygons and clumps (clusters) [22]. Clumps can be formed by adding two or more spherical particles together to form one rigid particle [23]. Particles within a clump can overlap to any extent and contact forces are not generated between these particles.

When laboratory setups are modelled in DEM, it might be possible to accurately model the size of the particles. However, when large scale industrial applications are modelled, it would normally not be possible to accurately model the particle size since it would be computationally too demanding. In order to decrease the total number of particles, it is possible to increase the particle size. It has been shown by Obermayr et al. [24] and Ucgul et al. [25] that particles can be scaled up in size and still the draft force in soil can be accurately predicted. For a review on the

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DEM modelling of non-spherical particles see Lu et al. [22]. In this study, however, the actual size of the particles was used to build the model particles.

There are two schools of thought in literature when it comes to the determination of the DEM input parameters [21]. The first approach is to make use of a calibration procedure where either in-situ or laboratory experiments are performed to measure a specific macro property. The experiment is then numerically replicated by following the laboratory or field setup and procedures as closely as possible. The micro parameter values are then changed iteratively until the predicted macro response matches the measured result. A potential problem with this approach is that the macro response of the numerical experiment can be influenced by more than one parameter. This means that there is no unique solution since more than one combination of the parameter values will result in the same macro behaviour. If this is the case, it is not to say that once the material is calibrated for one application it will be accurate for another. Also, the DEM models were developed by giving physical meaning to the parameters, but if this approach is followed, the physical meaning of the parameters might be lost [21]. The following authors made use of this approach to some degree.

Marczewska et al. [26] did not calibrate a specific material, but showed the effect of changing the contact stiffness and the friction coefficient on the bulk stiffness through triaxial tests on spherical particles. Lu and McDowell [27] developed a method to create clumps for ballast particles and showed that these particles performed better than spherical particles in terms of the sleeper load-displacement response. Huang and Tutumluer [28] used the direct shear test to determine both the contact stiffness and friction coefficient of ballast particles, although it had been shown by others that the shear box results were influenced by both of these parameters [11,29]. Li et al. [30] made use of triaxial experiments and a calibration procedure based on a response surface method to determine the stiffness and friction coefficient of rock fill material. Asaf et al. [8] proposed an in-situ method for determining the micro parameter values. Their method was based on wedge penetration tests and a non-linear optimisation scheme. Mak et al. [31] modelled soil-tool interaction and made use of an iterative process to obtain the DEM parameter values. However, they did not propose a general calibration procedure, but rather used the draft force on a blade to set the parameter values. Grima and Wypych [32–33] made use of direct shear tests and a newly developed slump-tester to determine the input parameter values of polyethylene pellets. Tanaka et al. [34] conducted bar penetration tests and compared the results with those obtained from DEM simulations. The contact stiffness was chosen without any experimental validation and by comparing the movement of the particles during the experiment with the movement of the particles during the simulation, the friction coefficient could be determined. Franco et al. [35] proposed an inverse calibration method to determine the micro parameter values. Based on DEM results, the particle friction coefficient and stiffness were determined from energy principles and direct shear tests. Derakhshani et al. [36] made use of spherical particles to model quartz sand. They determined both the particle sliding friction and rolling friction by modelling the flow of sand through a sandglass. They showed that two independent parameters were needed to be measured in order to determine a unique set of values for the two unknown friction parameters. For this purpose they used the angle of repose that formed as the sand flowed through the sandglass as well as the discharging time. Li et al. [37] followed a very similar approach. They too made use of spherical particles to model soybeans and showed that the angle of repose was a function of both the sliding and the rolling friction. The final set of calibrated parameter values had to satisfy both the angle of repose and the discharge time of a hopper. Simons et al. [38] made use of a ring shear tester to calibrate the micro parameters. They concluded that the sliding friction, the rolling friction and the particle stiffness had an effect on the results and that another experiment should be conducted to determine the stiffness. In this paper, the confined compression test was used to determine the particle stiffness, followed by the direct shear test to determine the particle–particle friction coefficient.

The second approach to determine the input parameter values is to directly measure the values on the particle level. Some of the parameters are easy to measure while others are very difficult, depending on the particle scale. Several attempts were made in literature, but they were all applied to particles in the millimetre and above size range [21]. Even if the micro parameter values can be directly measured, it does not necessarily mean that the DEM model would show the same level of accuracy on a macro level. This approach would only be accurate if the shape and size of the particles are modelled accurately and if the contact model is an accurate representation of the contact behaviour [39]. It is difficult to accurately model the particle size and shape when large industrial scale systems are modelled. The particle size often has to be increased [32] and the particle shape cannot be accurately modelled due to computational limitations. It is very difficult to accurately model the shape of most real particles unless the particles happen to be spheres [40–41] or specific simplified shapes tested in the laboratory. The advantage of this direct measurement approach is that the resulting micro properties are not dependent on the contact model or the specific DEM code used [42]. Very few researchers have tried to experimentally measure the micro parameters.

Vu-Quoc et al. [43] measured the coefficient of restitution in soybeans using drop tests and Gonzalez-Montellano et al. [44] measured the micro parameters of maize grains and olives and validated the procedure by modelling silo discharge [45]. Paulick et al. [46] developed a technique to measure the particle contact stiffness while eliminating the machine deflection. This was however only applied to spherical particles. Wang et al. [47] measured the coefficient of restitution of differently shaped maize particles using cameras. They concluded that the coefficient of restitution was dependent on the particle shape and also the angle of impact. Although their results were conclusive, it would be impractical to perform such tests as part of a calibration process for each particle shape and impact angle and equally so to implement in a DEM code. Barrios et al. [48] performed tests on a single iron ore pellet to obtain the necessary parameter values. They performed tribometer tests to obtain the friction coefficients, the rolling resistance was measured on an inclined plane and the coefficient of restitution was measured using a drop test. Validation was done by modelling the static angle of repose and the tumbling action inside a rotating mill. They concluded that the single-particle tests were viable for estimating the parameter values, provided particle shapes were described appropriately. However, if single spheres were used, the bulk behaviour no longer matched that of the experiments unless the parameter values were adjusted. If this was done, the physical meaning of the parameters was lost to some degree.

For the discrete element method to be successfully used by industry, a calibration procedure is needed for materials with relatively large particle sizes. Therefore the main objective of this study was to make use of a calibration procedure to determine all the DEM parameter values needed to model crushed rock with particles up to 40 mm in size. For this purpose, a large shear box was used. Special emphasis was also placed on the effect of the modelled particle shape. Different clump types were used and each was individually calibrated. This is important since the performance of different particle shapes cannot be compared if the exact same parameter values are used for all. If the modelled particle shape is changed, the parameter values should be re-calibrated to take this change into account. To validate the calibration process, the calibrated parameter values were used to model anchor pull-out tests where the pull-out forces were compared to experimental measurements and also hopper discharge where the discharge rate was compared to experimental measurements. The commercial DEM software package, PFC^{3D} (version 4.0), was used in this study [23].

Our approach was to perform laboratory experiments where the macro properties could be measured and then through a reverse calibration process, the experiments were repeated numerically to find