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Development and validation of calibration methods for discrete element modelling

Andrew Phillip Grima · Peter Wilhelm Wypych

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Abstract Discrete element method (DEM) is proving to be a reliable and increasingly used tool to study and predict the behaviour of granular materials. Numerous particle-scale mechanisms influence the bulk behaviour and flow of bulk materials. It is important that the relevant measurable input parameters for discrete element models be measured by laboratory equipment or determined by physical calibration experiments for rational results. This paper describes some of the bench-scale experiments that have been developed to calibrate the DEM simulations to reflect actual dynamic behaviour. Relevant parameters such as static and rolling coefficients of friction, coefficient of restitution and inter-particle cohesion forces from the presence of liquid bridges have been investigated to model the bulk behaviour of dry and moist granular materials. To validate the DEM models, the results have been checked against experimental slump tests and hopper discharge experiments to quantitatively compare the poured and drained angles of repose and solids mass flow rate. The calibration techniques presented have the capability to be scaled to model and fine tune DEM parameters of granular materials of varying length scales to obtain equivalent static and dynamic behaviour.

Keywords Discrete element method · Non-spherical · Calibration · Angle of repose · Cohesion

1 Introduction

The understanding of granular flows is of great importance in the industries that rely on bulk materials handling and processing. Continuous improvement and innovation in computer simulation software to analyse the performance of complex systems handling difficult granular products is required to improve process efficiency, reliability and assist in minimising the amount of waste material. Discrete element modelling is gaining interest in many industrial applications as a valuable numerical design and trouble-shooting tool for engineers. However, methods to accurately calibrate and numerically quantify the bulk mechanical behaviour of granular materials from measured properties are still a formidable task with many suspicions about the validity of measured parameters and the subsequent simulations.

There are numerous validated continuum methods which have proven to be accurate and reliable over the years to study confined and unconfined granular flow. Unlike conventional continuum mechanics, DEM can be time consuming to set up detailed models and can be limited by computational resources, which restricts the number of particles and the size of a system that can be analysed. The distinct advantage of DEM is the ability to model individual particle dynamics/transients and local interactions with other particles and equipment surfaces. The DEM code has advanced significantly to have the ability to model irregular particles of varying size distribution and mechanical properties. Non-contact particle forces such as capillary forces from liquid bridges [1] have successfully been incorporated into the DEM code to model a vast range of materials from dry fine powders to wet granular products. Numerous calibration and validation techniques have been previously investigated including granular pile formation [2] and direct shear tests [1,3]. Coetzee and Els [3] have examined various techniques to validate

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and select appropriate DEM model parameters to successfully model granular flow. This paper investigates alternative simple bench-scale experiments to directly "tune" or calibrate DEM model parameters and optimise computational time by scaling methods.

2 Bulk material properties determination

Determination of key parameters of a bulk material is essential when it comes to the analysis of granular flow using any numerical method. For this investigation various tests were conducted on dry and wet washed coal with a top size of 4 mm. These tests involved evaluating the particle size distribution (Fig. 1), solid and loose-poured bulk densities, particle shape, coefficient of restitution (CoR), static friction angle for particle-to-particle and particle-to-boundary interactions, tensile strength and bulk compressibility. Some of the experimental parameters are listed in Table 1. The CoR has been determined using a high-speed camera to analyse the velocity just before and after impact as shown in [4]. Two reasonably flat particles of varying size were placed securely on a plane and inclined to the point of slippage to approximate the static friction angle between particles and likewise for a boundary material.

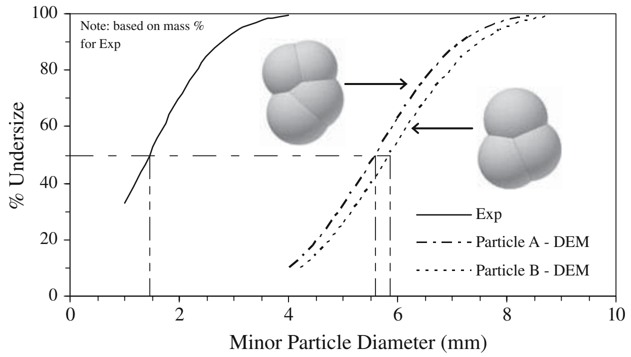

Fig. 1 Particle size distribution of washed coal and DEM scaled particles

Table 1 Measured properties of washed coal

Parameter	Value
Solids density, ρ_s $(\mathrm{kg\ m^{-3}})$	1,430
Loose-poured bulk density,	788 (Dry)
ρ_{bl} $(\mathrm{kg\ m^{-3}})$	662 (7.5% wb moisture content)
	646 (15% wb moisture content)
Coefficient of restitution (CoR)	0.55 (particle-to-particle)
	0.6 (particle-to-perspex)
Static friction coefficient (μ_s)	0.58 (particle-to-particle, dry)
	0.43 (particle-to-perspex, dry)

3 Setup of calibration apparatuses

To provide experimental data of granular flow and behaviour several bench-scale tests have been developed to examine the mechanics of granular flow in various conditions and confinements. The aim of these tests is to assist in the calibration of numerical parameters required for DEM simulation using numerous experiments to isolate key properties such as particle-to-particle static and rolling friction coefficients. Once a suitable parameter is determined other interactions can be additionally investigated including extra boundary materials, cohesion and alternative dynamic interactions, such as multi-phase analysis and other non-contact environmental conditions (e.g. electrostatics).

A common test to study the influence of particle friction and rolling resistance on the formation of granular piles is a slump test where material is loosely poured into a tube and lifted to allow material to form a pile under gravitational forces. This is used primarily to examine the angle of repose and pile height. The disadvantage of this arrangement is that as the tube is lifted at a set rate the flow of material is influenced by friction between the particles and the tube wall and the lifting velocity. To avoid these affects an alternative slump tester has been designed as shown in Figs. 2 and 3, where a perspex split tube is filled with material and released by the two halves pulling away laterally from each other around a fixed point in an arc. High-speed photography has shown that the two halves pull away quickly enough to avoid any contact with the bulk material as shown in Fig. 3. A pipe filled with granular material to form a flat surface under the slump tester is an effective method to solely calibrate the particle-to-particle interactions as other interactions are negligible. Once the pile is formed the profile can be quantified using the angle of repose and the contour of the pile. For this investigation a 60 and 100 mm inside diameter (I.D.) tube has been used to examine the effects the aspect ratio of the column of

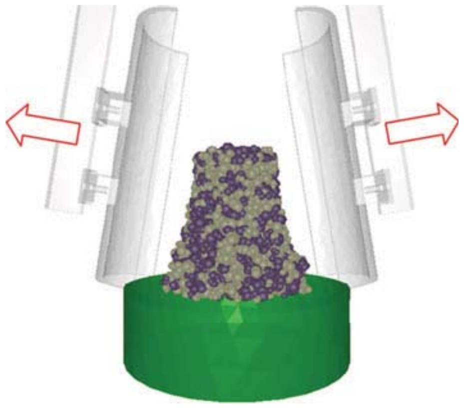

Fig. 2 DEM model of swing-arm slump test after release. 60 mm I.D. tube, 150 mm I.D. base

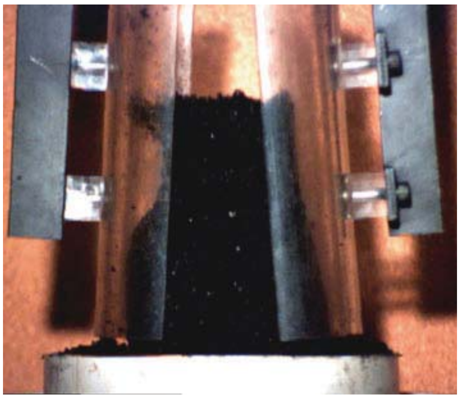

Fig. 3 Swing-arm slump tester after release. 60 mm I.D. tube, 150 mm I.D. base

material may have on particle flow and pile formation during slumping.

To verify that the parameters obtained from the slump test (i.e. unconfined flow) are suitable for confined flow, a test apparatus was set up consisting of an adjustable perspex flat-based hopper elevated 200 mm above a flat load platform supported by a load cell as shown in [4]. With an adjustable opening and a quick release gate the material discharge rate can be varied to examine the drained angle of repose, different flow behaviours and phenomena that may occur such as cohesive or mechanical arching. The influence that drop height has on the formation of a granular pile in comparison to the piles formed by slump testing can also be examined. The profile of the material discharging from the hopper and the duration of discharge can be recorded by a high-speed camera to compare with numerical models and determine whether the particle dynamics and contact physics are representative on a macro scale.

Conducting a variety of physical tests enables a database of information to be collected to assist in the selection of appropriate parameters and material mechanical properties for various environmental conditions, applications and numerical optimisation. It is not expected that DEM parameters determined from one type of experiment will be realistic to characterise the dynamics of a bulk material in general. Fine adjustment of parameters, including particle shape may be required to achieve an accurate representation of bulk behaviour from observations from various bench-scale experiments.

4 Numerical modelling

DEM is an effective tool to simulate granular flow of dry and moist materials. The commercial code utilised in this study is EDEM [5]. The simplified non-linear visco-elastic Hertz-Mindlin no-slip model was adopted in the present work. Further details on this contact model are provided in [6]. To account for surface asperities and particle geometry which can not be easily modelled in DEM simulations, rolling friction was necessary to apply a resisting rolling torque to oppose the relative rotation between particles and between particles and boundaries. A simple Coulomb-like rolling friction model proposed by Zhou et al. [2] was implemented in addition to using shaped particles. Additionally, to appropriately model the capillary forces and cohesion between particles in wet granular materials, a simple approach affiliated with the EDEM code [5] has been adopted that increases the normal contact force proportionally to the normal particle overlap and subsequently increasing the tangential contact force. According to Hertz theory of elastic contact [7], the contact area radius can be evaluated by:

$$r^2 = 2R \cdot h \tag{1}$$

where R is the particle radius and h is the normal overlap. The additional normal repulsive force is expressed as:

$$F_N = \pi r^2 C_e \tag{2}$$

where C_e is cohesive energy density $\left(\mathrm{J\ m^{-3}}\right)$. An approach adopted in this investigation to approximate the cohesive energy required to simulate tensile strength in moist materials is based on the general formula derived by Rumpf [8] to originally calculate the tensile stress of wet mono-sized spherical particles. With an empirical correlation for the coordination number the tensile stress is related to the following expression:

$$\sigma_N = \frac{1-\varepsilon}{\varepsilon}\frac{F_N}{d^2} \tag{3}$$

where ε is the voidage of the granular material dependent on the consolidation stress, F_N is the bonding force of a liquid bridge and d is the particle diameter. Figure 4 provides a comparison between the minor principal tensile stress (i.e. perpendicular to the axis of consolidation) of washed coal at 7.5 and 15% wet basis (wb) moisture content measured with an Ajax tensile tester [9]. The cohesion energy is also estimated using Eqs. 2 and 3 in Fig. 4 to provide a preliminary guide to the selection of the correct additional force required to represent moist bulk material under various consolidation conditions.

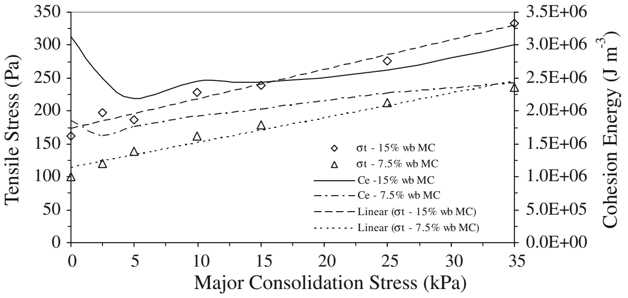

Fig. 4 Tensile stress and cohesion energy vs. major consolidation stress for moist washed coal: h ≈ 0.1µm, d = 5 mm

To represent particle shape two different simple particle shapes were created by clustering spheres, as shown in Fig. 1. The mean particle size was approximately scaled up by a factor of 4 to reduce the number of particles required and the simulation time. As no indentation or compression tests were conducted to determine the stiffness of the washed coal, the modulus of elasticity and Poisson's ratio were approximated at 2.43 GPa and 0.35, respectively.

A series of simple simulations were conducted to quantify the CoR of the shaped particles and spherical particles by dropping the particles in a fixed orientation onto a flat surface. Comparisons of the impact and rebound velocity showed that the CoR for spherical particles correlated well to the input value unlike the shaped particles where the average simulated CoR was lower than the input value. As energy is absorbed by rotational motion when two or more spheres of a clustered particle collide within a short period resulting in an oblique impact, adjustments were made to the measured CoR by increasing the particle-to-particle and particle-to-perspex CoR to 0.78 and 0.8, respectively. Increasing the CoR reduced the difference between the numerical rebound velocity of shaped particles and the measured rebound velocity of the coal particles. The sensitivity of the CoR on modelling granular flow using non-spherical particles with low relative collision velocities is also examined in this paper.

5 Results and discussion of slump tests

From a practical point of view, it is ideal if appropriate parameters for a DEM model can be evaluated in the shortest period possible to minimise the cost of computational and human resources. The approach adopted to minimise computational time was to set the particle-to-particle friction to the measured static friction coefficient ($\mu_s = 0.58$) and arbitrarily adjust the rolling friction coefficient (μ_r) accordingly until the pile closely matched the experimental measured profile. The static friction coefficient and CoR were also adjusted to examine the effects they had on the particle flow. For the dry washed coal there was some difference between the angle of repose and the pile height using a 60 mm I.D. tube (Fig. 5) and a 100 mm I.D. tube (Fig. 6) filled with material to a height of 150 and 100 mm, respectively. The reason for the differences is due to the difference in the potential energy of the systems resulting in different average particle velocities during the slump tests.

Initially, μ_r was set to 1% of μ_s, however this was not sufficient even with high values of μ_s. Increasing μ_r resulted in significant changes in the pile height compared to increases of μ_s that governed more the angle of repose. Figure 5 shows greater increases in pile height with changes in μ_r and μ_s, unlike Fig. 6 where the increases result in minor changes in pile height. The effect that the CoR has on the angle of repose and the pile height is minor at relatively low collision velocities. To select which set of parameters best depicts the bulk material behaviour a comparison is made between the different slump tests and the bulk density measured when the particles are loosely injected into the tube prior to the slump arms being released. Referring to Fig. 6 the measured bulk densities for each DEM simulation were 819 (DEM 1), 810 (DEM 2), 799 (DEM 3) and 777 kg m^{-3} (DEM 4). Thus the set of particle parameters which best complies with the profiles and bulk density is $\mu_s = 0.6$, $\mu_r = 0.1$, CoR $= 0.78$ or 0.55.

Utilising the parameters determined for free-flowing dry washed coal the effects that adhesion and cohesion have on flow were investigated to determine how much cohesion energy is required to represent the liquid bridges between the particles. Figures 7 and 8 show the DEM and experimental profiles of the granular piles formed from moist washed coal with varying moisture content and strength. Using the approximated values of cohesion energy from Fig. 4 the DEM

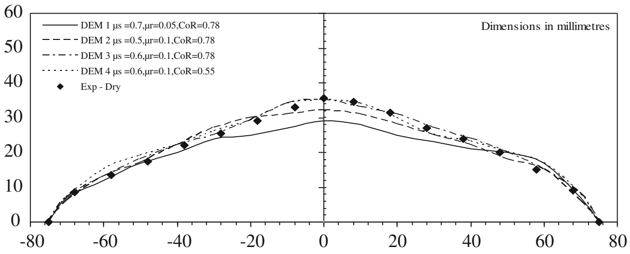

Fig. 5 Granular pile profiles for dry washed coal from slump test: 60 mm I.D. tube, 150 mm initial fill height in tube

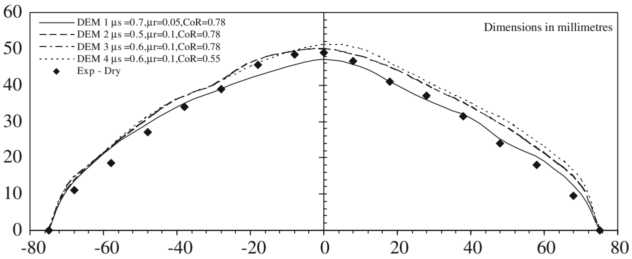

Fig. 6 Granular pile profiles for dry washed coal from slump test: 100 mm I.D. tube, 100 mm initial fill height in tube

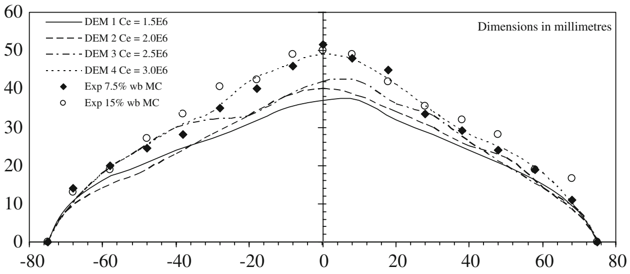

Fig. 7 Granular pile profiles for moist washed coal from slump test: 60 mm I.D. tube, $\mu_s = 0.6\,\mu_r = 0.1$ CoR=0.78, 150 mm initial fill height in tube

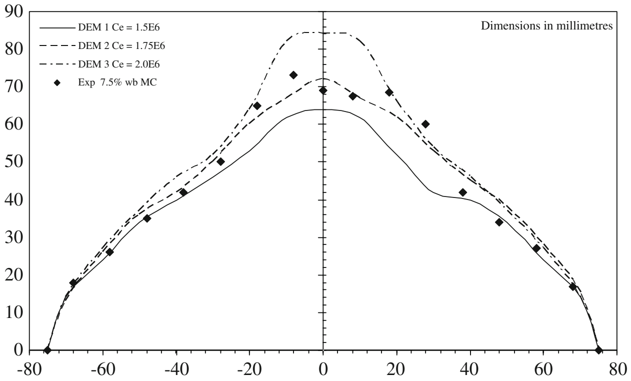

Fig. 8 Granular pile profiles for moist washed coal from slump test: 100 mm I.D. tube, $\mu_s = 0.6$, $\mu_r = 0.1$, CoR = 0.78, 100 mm initial fill height in tube

simulations and experiments were conducted using a similar manner where the initial height of material in the tubes was identical. Figure 7 shows that the experimental profiles for washed coal at 7.5 and 15% wb moisture contents were very similar in regard to pile height and angle of repose. With the addition of 3×10^6 J m^{-3} of cohesion energy to the particle contacts the behaviour of the material slumping correlated well to the physical behaviour of the washed coal at 7.5 and 15% wb moisture content from the 60 mm I.D. tube slump test. A clear distinction in the height of the piles between the dry and moist washed coal can be seen when comparing Figs. 5 and 7.

The unconfined strength of the moist washed coal was noticed when the bulk material did not fail successfully when washed coal with a moisture content of 15% wb was loosely poured into the 100 mm I.D. tube to a height of 100 mm in the swing-arm slump tester. However, at half the moist content the material successfully failed and formed a pile as shown in Fig. 8. A cohesion energy of approximately 1.75×10^6 J m^{-3} is required to model the flow behaviour of washed coal with a moisture content of 7.5% wb in the 100 mm I.D. tube slump test which is significantly different from the 60 mm I.D. tube slump tests. Between the 60 and 100 mm I.D. tube slump tests the deviation between the particle dynamics and the total system energy result in marginally different particle normal overlaps in the DEM simulations which govern the magnitude of the additional cohesive normal force added between particles during a collision. Consequently, a cohesion energy determined suitable for one system may not be suitable for another system. As it is complex to model transferable liquid bridges in DEM, the bulk density measured experimentally decreases with increasing moisture content, however in the DEM simulations shown in Figs. 7 and 8 the bulk density of the moist material varied between 715 and 793 kg m^{-3} which is greater than the measured values in Table 1.

Adjustments could be made to the solid density of the particles to artificially modify the bulk density, however this will alter the gravitational weight forces on the particles. The unsuccessful failure of the column in the 100 mm I.D. tube of the slump tester was successfully simulated numerically when the cohesion energy between the particles was greater than 3×10^6 J m^{-3}, showing that calibration of adhesion and cohesion in a granular material is dependent on the consolidation state and environmental conditions. However, the evaluation of the cohesion energy via Rumpf's expression (Eq. 3) has shown to be a plausible method to approximate the required additional particle tensile forces to replicate physical particle mechanics for moist materials.

6 Results and discussion of discharge from hopper

To verify that the results obtained from the slump tests are valid for confined flow various tests were conducted using dry washed coal to examine the behaviour of material discharging from a hopper. As the hopper has a flat base and no sloped walls the particle-to-particle interactions could be examined with minor influences from the hopper walls. Using the suitable parameters established in the slump tests, numerous DEM simulations of the hopper flow for dry washed coal were conducted. Investigations found that a minor decrease in the particle rolling friction coefficient to $\mu_r = 0.05$ achieved similar behaviour to the physical experiments. Figure 9 shows a good comparison between the simulated and experimental drained angle of repose in the hopper with a discharge opening of 40 mm. The discharge time between the experimental and numerical tests were within 15% of each other where μ_r had the greatest influence on the drained angle of repose in the hopper and the pile formed below the hopper. The discharge characteristics of the dry washed coal are shown in Fig. 10 which indicates that the washed coal is a free flowing material when dry as the change of the normal force on the load platform is quite rapid once the hopper gate opens. Figure 10 also shows the difference between the total normal forces exerted on the load platform below the hopper in the DEM simulations compared well to the experimental force.

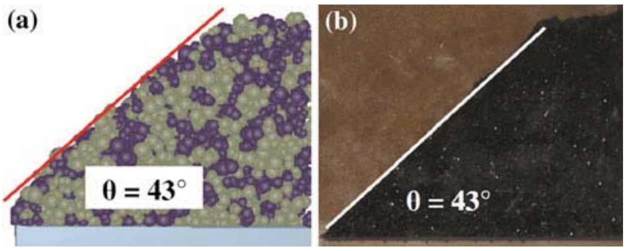

Fig. 9 **a** DE model of angle of repose at discharge point in hopper: $\mu_s = 0.6$, $\mu_r = 0.05$, CoR = 0.78 and 0.55, **b** experimental profile of dry washed coal: 40 mm opening

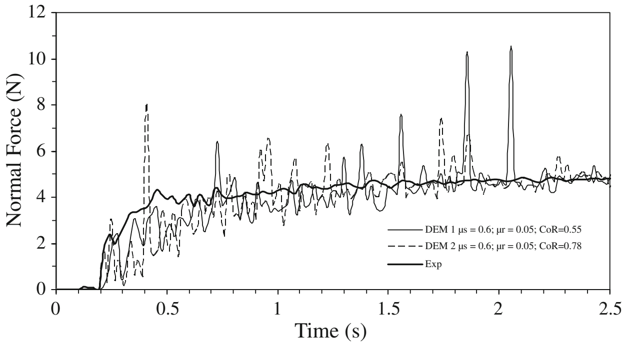

Fig. 10 Force exerted on load platform below hopper. Gate opens at time = 0 s

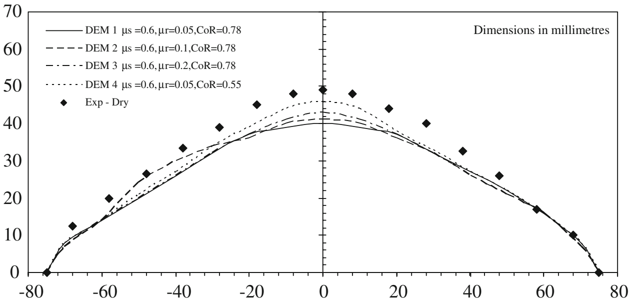

Fig. 11 Granular pile profiles for dry washed coal from hopper: 200 mm drop height

The profile of the granular pile formed below the hopper for dry washed coal is shown in Fig. 11. The difference between the piles in Fig. 11 is minor and the angles of repose are similar for various alterations in μ_r, however the set of parameters which best matched the angle of repose in the hopper and on the pile was $\mu_s = 0.6$; $\mu_r = 0.05$; CoR= 0.55. Although these parameters are slightly different to slump test parameters, this implies that DEM parameters have to be "tuned" according to the environmental conditions and application.

7 Conclusion

Numerous methods were presented in this paper to assist in the calibration process to determining the material parameters needed in DEM simulations. Numerical results for both cohesionless and cohesive granular materials were compared to experimental data to validate the DEM parameters such as the static friction coefficient, the rolling friction coefficient and the CoR. The developed techniques have proven to be successful for the calibration of material parameters but also allow for scope to optimise simulation time by scaling parameters such as particle size and particle stiffness. It is shown that DEM can accurately model the flow of granular material from discharge of a hopper and the formation of granular piles from slumping. The best method to tune DEM models to optimise time was to measure as many single particle properties as possible to develop an appropriate particle shape representation and size distribution. Once key parameters are determined, several simple experiments which best replicate the flow mechanisms of the system to be modelled can be conducted using a trial-and-error process where minimal dependent parameters are altered such as the rolling friction or cohesion energy as presented. Minimising the number of types of particle interactions to calibrate during a single experiment is ideal to effectively reduce the number of parameters which influence granular flow and the quantity of trial DEM simulations required. Other notable observations from this study is that the CoR is not so influential on the bulk behaviour during slump tests and hopper discharge, thus the adjustments made to the CoR to account for the effects of clustering spheres was not critical. Scaling up the average particle size to reduce computational time and the required number of particles proved to be plausible for unconfined flow but shows a tendency to restrict the flow of particles from a hopper which may be problematic for realistic flow of large models. Further investigation is being conducted to access the validility and accuracy of the bench-scale calibration techniques to model large-scale granular flow.

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