Discrete element model calibration for industrial raw material simulations

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Abstract. The use of computational fluid dynamics in continuous operation industries have become more prominent in recent times. Proposed system improvements through geometric changes or control strategies can be evaluated within a relatively shorter timeframe. Applications for discrete element methods (DEMs) in real life simulations, however, require validated material-calibration-methods. In this paper, the V-model methodology in combination with direct and bulk calibration approaches were followed to determine material model parameters, to simulate real life occurrences. For the bulk calibration approach a test rig with a containment hopper, deflection plate and settling zone was used. Screened material drains from the hopper, interacts with the deflection plate, and then settles at the material angle of repose. A high-speed camera captured material interaction with the rig, where footage was used during simulation validation. The direct measuring approach was used to determine particle size, shape and density, while confirming friction and restitution coefficients determined in the bulk calibration method. The test was repeated and validated for various geometrical changes. Three categories of validation were established, namely particle speed assessment, -trajectory assessment and -plate interaction assessment. In conclusion, the combination of direct and bulk calibration approaches was significant in calibrating the required material model parameters.

1 Introduction

The relevance and application of discrete element methods (DEMs) in industry has increased significantly in recent years. The use of an accurately calibrated model decreases the time required for studies into operational and design changes. In particular, these models aid in identifying root causes for reduced efficiency and/or equipment life without physically interfering with plant production. This reduces the total cost of the investigation when compared to the conventional trial and error approach [1].

A DEM is normally used in studies where the importance of identifying bulk material behaviour is important [2]. Therefore, DEMs are typically applicable to production industries, and more specifically, the steel industry.

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Within the steel industry, iron making is the process of converting raw materials into molten iron. This is typically done through a blast furnace, where raw material is loaded from the top whilst hot air and pulverised coal is injected and combusted at the tuyeres, just above the hearth [1].

The raw materials that are typically a calculated mixture of metallurgical coke, sinter, ore and additives, are loaded into the top of the blast furnace via 2 methods; 1) a skip loading system and 2) a conveyor loading system [1]. With the conveyor loading system, hoppers are filled with their designated materials and then drained by loading the material onto a continuously moving steep inclined sidewall conveyor. This conveyor then transports the material to the top of the blast furnace for discharge. Some of the process problems that typically occur at this loading point is constant spillage and abrasion wear on belt edges.

The bulk coke material handling internal to the iron making process was identified as a possible case study. This study will demonstrate that a DEM is capable of simulating the bulk material behaviour when coke is discharged from a hopper onto a steep inclined sidewall conveyor.

There are numerous software packages that can be utilized in a study relating to a DEM. Simcenter STAR-CCM+ software package is used in this study due to the coupling of a DEM into a multiphase environment being readily available to the user [3].

2 Literature Survey

A paper by Coetzee [4] was aimed at critically evaluating different validation and model calibration techniques and determining if there is a definite model parameter or technique to be used for the most accurate results. The parameters evaluated were: particle shape, size, density, stiffness, rolling resistance, inter-particle and boundary friction coefficients (both static and dynamic), coefficient of restitution, cohesive properties and adhesive properties.

Thompson [5] investigated the calibration of different DEM model parameters for dry and wet granular materials, in order to determine if the model is capable of replicating material bulk behaviour. Marigo and Stitt [6] used a rotating drum as a validation mechanism for a DEM model developed for the evaluation of the influence that the detail of the particle shape has on bulk material behaviour. The only parameter that [6] identified as critical in addition to those mentioned by [4] was the Poisson's ratio.

Grima and Wypych [7] investigated the sensitivity of the variation of various DEM parameters on the impact reaction force of polyethylene pallets on a plate. This study attempted certain scaling rules in order to reduce the number of particles in the domain and in doing so minimise the computational time.

Further, Horn [8] conducted a study on the calibration of relatively large ore aggregate particles by using a large-scale shear box. The parameters identified to be critical in addition to those mentioned by [4] [5] and [6] was bulk density, material porosity, Young's modulus and the internal friction angle. This study used small scale tests for validation of the calibrated DEM model and it was concluded that the model replicated the material bulk behaviour within an acceptable margin.

3 Experimental Setup

The design of the test bench and the calibration methodology was based on work by Quist and Evertsson [9]. The referenced study was aimed at developing a calibration framework that would not only assist in validation but also ensure accuracy of results.

Figure 1: Test rig setup used in this study

The calibration framework developed by [9] and referred to as the “V-model” comprised of three levels, each linking between the simulation and experimental domains. The calibration process starts at the first level, which is the single property lab test. This level correlates with the direct measuring approach of [4]. These properties are then included in the simulation domain and a first level validation is done.

The second level is defined by multiple flow regime experiments. This level determines if the bulk flow behaviour produced by individually calibrated parameters correspond within a degree of accuracy to an experimental test. This level correlates well with the bulk calibration approach of [4]. It is a common occurrence in this level to find that the parameter adjustments are required before the model correlates well with the experimental results. It is advised that during this stage, the experimental setup should be altered to ensure there is still an acceptable degree of accuracy between the experimental and simulation domain [9].

The third level is defined by an industrial scale experiment. For this level the model parameters are validated further with actual material handling processes. At this point, it can be determined if the model parameters are within an acceptable region of accuracy and thus deemed calibrated.

The relevant experimental setups to determine the parameters mentioned in the literature survey can typically be categorized into two approaches; the *Bulk Calibration* and *Direct Measuring* approach [4].

Table 1: Approaches to determine DEM parameters used in this study [4]

Bulk Calibration Approach	Direct Measuring Approach
Coefficients of Restitution (Particle-Boundary)	Particle Shape
	Particle Size
Static Friction Coefficient (Particle-Particle)	Particle Density
	Static Friction Coefficient (Particle-Boundary)

4 Parameter Calibration

4.1 Direct Measurements

4.1.1 Particle Size

Throughout literature the size of the particles in the DEM simulation is considered as an important parameter that has to be included in the calibration of the model. In most cases the size of the particle has to be scaled up to reduce the number of particles in the simulation so that the computational time can be reduced.

Roesller and Katterfield [10] stated that the total degrees of freedom are affected when the particles are scaled and that the scaled particles should be calibrated with regards to the material bulk behaviour. In laboratory simulations with a small number of particles it is possible to size the particles closer to the actual value, but when industrial size simulations (typically hopper or silo discharge) are simulated, the user is forced to reduce the number of particles in the simulation.

Shigeto et al. [11] investigated the influence of scaling up fine power particles for a screw conveyor application. In this report spherical particles were used and it was found that particles could be scaled up to 4 times while still producing accurate material bulk behaviour.

Grima and Wypych [7] determined that care should be taken when scaling rules are applied to particles when impact force is evaluated. The authors concluded that the size of the particles had an effect on the resolution of the result and therefore if the particle scaling was too great a variation in the impact area would be obtained [7].

Xie et al. [12] used a similar conveyor design set up as [7] in order to investigate the wear process of a conveyor transfer chute. It was concluded that the particle size should not be scaled by more than a factor of 2 when conveyor transfer chutes are modelled.

Measurement

Coke particles were obtained and screened according to normal processes. Additional screening was required due to size limits on the experiment test rig. The following size distribution was obtained:

Table 2: Particle size distribution obtained for experiment

Particle Size Distribution of Coke						
	>100 mm.	80-100 mm.	60-80 mm.	40-60 mm.	35-40 mm.	30-35 mm.
% Coke per size	0%			83%	11%	6%
Modelled Size	80mm			60mm	40mm	35mm

4.1.2 Particle Shape

The most common particle that is used when setting up a DEM analyses is a spherical particle shape. This is due to a spherical particle shape providing sufficient contact detection criteria which allows the solving time of the simulation to be reduced [13].

The study of [13] investigated the difference in DEM parameters when spherical clumps of 2, 4 and 8 spheres were used. It was concluded that a manually generated spherical clump particle replicated the material behaviour more accurately than a single sphere particle.

Pasha [14] investigated the difference in modelled bulk material behaviour if spherical particles with an additional friction factor are used vs. optimised particle clumps without a

friction factor. It was stated that particles comprising of 5 spheres in a clump will be able to produce adequate results for material bulk behaviour [14].

Markauskas and Kacianauskas [15] developed a particle simulation with the use of a hopper draining test and simulated particles shaped like axisymmetric clumps. It was found that even though the shape closely resembled the actual particles, the model still required some calibration with regards to other parameters in order to accurately replicate the material bulk behaviour [15].

Measurement

For the particle shape calibration, 14 random particles were selected from the screened samples. The particles were placed on a grid representing a 60mm x 60mm block. A photo was taken and imported into a CAD program after which representative shapes could be drawn on scale. The result is shown in the figure below.

Figure 2: Visual shape analyses

It followed that most particles could be represented by a triangular cluster of spheres, and for simulation purposes it was therefore decided to follow this modelling approach. The size distribution of the simulated particles was obtained by changing the diameter of the spheres within the cluster according to the total particle diameter required.

Figure 3: A modelled particle in STAR-CCM+

4.1.3 Particle Density

In industry, material density is generally defined as the bulk density. The bulk density is defined as the mass of a sample per unit volume.

Horn determined the specific particle density of a medium size ore aggregate (40mm) by measuring the volume of water being displaced when a known mass of material was submerged in the container [8]. The bulk density was then determined by filling the large-scale shear box tester volume with the material, measuring the mass of the container and dividing it by the known volume of the shear box tester container. Additional properties like the void ratio and porosity were then calculated with the use of the particle density and the bulk density. These values were then used for the calibration of the DEM particle density.

Measurement

Since the volume of a particle could not be calculated as easily as the mass of the particle, a test setup was required. A particle sample is submerged in water whilst the displacement of the water is measured. The assumption is made that the particles don't absorb water. From the assumption, the volume of the coke particle is equal to the volume of displaced water.

The results from this test are given in the table below:

Table 3: Particle density calculation

Particle Density Calculation		
Weight of Container	0.390	kg
Weight of Material without Container	1.328	kg
Volume of water without material sample	0.003	m ³
Calculated volume of material	0.001	m ³
Particle Density	1021	kg/m ³

The calculated particle density was determined to be 1021 kg/m³. This was determined to be within the typical range for coke (800-1200 kg/m³) processed at this specific plant. Therefore, this value was deemed accurate for modelling purposes.

The solid material bulk density is defined by [8] as the mass of the sample divided by the volume which the material occupies. From this definition it is clear that the bulk density also includes the voids that are present between the particles as illustrated by Figure 4.

Figure 4: Bulk volume, voids volume, solid volume

In order to calculate the bulk density, the sample was placed within a known volume and weighed. The bulk and particle densities are then used to determine the void fraction e , and porosity n , by using the equations below;

$$e = \frac{\rho_p}{\rho_b} - 1 \tag{1}$$

$$n = 100 \left(\frac{e}{e + 1} \right) \tag{2}$$

The bulk density was determined to be 428.4 kg/m³, with the void fraction and porosity being 1.39 and 58.1% respectively. These values were within the 400-600 kg/m³ design limits.

4.1.4 Particle-Boundary Friction Coefficient

The particle-boundary friction coefficient is a parameter that is used to describe a particle's resistance against motion when it is in contact with a boundary surface. Failure to calibrate this value correctly will lead to errors in drainage time and the velocity of particles exiting the hopper.

Research performed by [8] determined the particle-boundary friction coefficient by placing a particle on the surface of the boundary to be assessed. The boundary surface was

then lifted until the particle started to slide. The angle (θ) at which the particle slid was then recorded and a friction coefficient (μ_b) was calculated with the use of this angle and the equation below.

$$\mu_b = \tan(\theta) \tag{3}$$

Measurement

The deflector plate of the test rig is used for this calculation. Due to the nature of the problem to be modelled, only 2 materials are included in the boundaries. These are the rubber (conveyor material) and liner plate (liner in coke hopper).

These materials are individually fastened to the test rig deflector plate after which a particle is placed on the plate. The deflector plate is rotated until the particle starts to slide. The angle at which the particle slides is recorded with a protractor. The test is repeated 20 times and an average particle-boundary coefficient was calculated for the interaction between coke-conveyor and coke-liner.

Table 4: Particle-boundary friction coefficient results

Particle-boundary friction coefficient results		
Material	Average angle deg.	Average friction coefficient
Rubber	40.23	0.852
Ceramic liner plate	13.5	0.240

4.2 Bulk Calibration

4.2.1 Coefficient of Restitution

The coefficient of restitution is a parameter used in DEM to illustrate the damping mechanism which occurs when a particle makes contact with a boundary surface or another particle.

When no viable test is available to determine the coefficient of restitution between particles, it is recommended to that a default value of 0.3 should be used when simulating hard rock ores [5].

Some researchers followed the drop test to determine the coefficient of restitution but when particles with varying shapes are used a reverse calibration technique was followed [4]. Thus, a simulation model was set up and the coefficient of restitution was changed until it matched the actual drop test result.

A drop test consists of a particle being secured at a known height above the boundary material. The particle is dropped and allowed to bounce on the boundary material while the movement is captured with a high-speed camera. The height the particle obtains after contact is then measured which is then used to calculate the velocity directly after contact. It is assumed that air resistance does not have a significant effect on the particle velocity. This enables the use of equation below for determining the velocity after contact.

$$v_f^2 = v_i^2 + 2g(x_f - x_i) \tag{4}$$

Measurement

An actual material particle does not have an exact spherical shape. To overcome this issue, particles were assessed in order to find the most spherically shaped particles.

The bottom deflector plate was positioned horizontally with a grid fastened to the back plate that consisted of 20x20 mm. blocks printed over the entire area. This grid will enable

the measurement of displacement height achieved after impact. This test was only completed for rubber material since the bounce mechanism is not required for the interaction between particles and the chute liner. The particle is released from the trap door position by hand to ensure the motion of the particle is not influenced by the trap door.

Figure 5: Experimental setup for coefficient of restitution calibration

For the simulation model, a similar setup in terms of geometry and drop position was made. The restitution coefficient is changed between tests, whilst a maximum velocity report measures the particle velocity throughout the drop test. The maximum velocity after impact of each coefficient of restitution is recorded.

By noting the maximum velocity after the simulated particle impact, a comparison can be made with the initial velocity calculated from the drop test results. The coefficient of restitution can then be calculated by determining the value at which the simulation and experimental domain deliver similar velocity results.

The drop test was repeated 10 times of which the average results are tabulated below along with the simulation model results.

Table 5: Coefficient of Restitution experimental and simulation results

Coke-Rubber velocity calculation result				
Experimental results			Simulation Results	
Particle displacement after impact	0.14	m	CoR = 0.2	0.688 m/s
Gravity	-9.81	m/s ²	CoR = 0.4	1.024 m/s
End velocity	0	m/s	CoR = 0.6	1.726 m/s
Initial velocity after impact	1.657	m/s	CoR = 0.8	2.454 m/s

As expected, with an increase in the coefficient of restitution, the initial velocity after impact is increased. By analysing the results, it can be determined that a coefficient of restitution of 0.6 will deliver sufficiently accurate results. Note that the value of 0.6 is used for both the normal and tangential components of the interaction since a spherical particle interaction was modelled.

As stated by [5], there is yet to be a test developed that will provide sufficient results for a particle-particle restitution coefficient. According to [5], a typical value for granular material is 0.3 for both the normal and tangential restitution coefficients.

4.2.2 Particle-Particle Friction Coefficient

The particle-particle friction coefficient is a parameter that is used within the DEM analyses which dictates the particle’s resistance against sliding when in contact with another. This is a parameter which is not easily measurable and is also reliant on other parameters.

For instance, if a sample of raw material is illustrated via spheres in a DEM analyses these particles will not experience the same interlocking characteristics due to the difference in shape. This parameter is therefore used to simulate a restriction in the movement so that the spherical particles replicate the actual material bulk behaviour.

Measurement

The experimental procedure consisted of a screened batch of coke particles being loaded into a containment hopper which is then drained through the trap door. The particle interaction with the deflector plate is then assessed. The entire draining process is recorded with a high-speed camera and the angle of repose formed at the bottom of the rig is measured.

A geometrically similar simulation model was setup with the calibration parameters determined in section 3.1 whilst the particle-particle friction coefficient was varied until the simulation model matched that of the experimental test.

Figure 6: Hopper draining simulation

The following results were obtained from repeating this test 5 times.

Table 6: Hopper draining test results

Hopper draining test		
Test number	Draining duration	Angle of repose
1	1.872 s	33 degrees
2	1.920 s	40 degrees
3	2.448 s	31 degrees
4	1.968 s	35 degrees
5	1.750	36 degrees

By analysing the hopper draining time in the simulation with the range of friction coefficients assigned, it was concluded that the friction coefficient does not have a significant effect on the hopper draining time.

The second portion of this section was to evaluate the effect the friction coefficient has on the angle of repose. The image of simulation result was captured and imported into a CAD program which allowed the measurement of angles.

Figure 7: Angle of repose vs friction coefficient

From the figure above, it is clear the angle of repose is influenced by the particle-particle static friction coefficient. Coetzee [4] stated that the angle of repose will start to flatten out, implying that there is a point at which the static friction coefficient would no longer have a significant effect on the angle of repose.

Coetzee [4] suspected that this point was reached, after which 2 additional simulations were done with a 3.5 and 4.5 static friction coefficient for confirmation. As shown in the figure above, this was indeed the case.

By comparison, it is evident that a particle-particle static friction coefficient of 2 matches the experimental results the best.

5 Final Validation

As stated by [9], a final parameter validation has to be done whereby the test rig settings should be adjusted to verify that the simulation still produces a similar result to that of the experimental test.

For this validation, it was decided to adjust the deflection plate to the extreme scenario a horizontal position. It is the furthest point from the initial calibration settings used and would thus be a clear indication of the model parameters are correct.

Figure 8: Final validation simulation model vs experimental model

The experimental test was repeated 3 times and recorded with a high-speed camera. The hopper draining time as well as the angle of repose formed on the deflection plate was measured and average across the 3 tests.

The table below is a summary of the results;

Table 7: Validation test results

Validation test results assessment			
Parameter	Experimental	Simulation	Deviation
Angle of repose (left)	44.57 deg	43.04 deg	-3.55 %
Angle of repose (right)	35.33 deg	32.87 deg	-7.49 %
Hopper drain time	1.8 0 s	1.44 s	0.36 s

The hopper draining time deviation of 0.36 s. corresponds with the findings in 4.2.2 and is thus deemed acceptable. The simulation model also, on average, produced a lower angle of repose for both the left and right side; 3.55% and 7.49% respectively.

From the results it can be concluded that the combination of direct and bulk calibration approaches is significant in the calibration of the required material model parameters.

6 Conclusion

In this paper a combination of the direct calibration and bulk calibration approaches were used to calibrate the material parameters for the Hertz Mindlin contact model. The direct measuring approach was used for the calibration of particle size, shape, density and boundary friction coefficients.

A test rig was built for the bulk calibration approach according to the calibration work done by [9]. The test rig was used for the calibration of the particle-particle static friction coefficient and the boundary coefficient of restitution. The test rig was also used for the final parameter validation and it was determined that the calibration process was applicable in producing a simulation result, which matched the experimental result.

The model accuracy obtained from combining the direct and bulk calibration methods justifies its use in building industrial models related to bulk material handling. The impact of design and operational changes can be quantified without stopping the industrial process. It also enables an iterative design process with the goal of maximising production and the operational life of components.

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