Calibration Procedure of Discrete Element Method (DEM) Parameters for Cohesive Bulk Materials

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Abstract

The downtimes are often too late to prevent the downtime of the system. One of the newer methods which can associated with blockage events in the materials handling sector is prompting the iron ore industry to optimise their operations to maximise the profitability of fines and lump products. These blockage events are caused by materials with high clay and moisture contents typically referred to as Wet and Sticky Material (WSM). There are numerous methods which are commonly used to prevent such blockage events, however, for majority of cases they be used to predict and visualise bulk material flow is the Discrete Element Method (DEM). DEM is capable of replicating the flow of non-cohesive granular materials with reasonable accuracy, however, when cohesive materials are considered the mechanism becomes much more complex. With the advancement of computational power over the last few decades it is now more practical to simulate WSMs into DEM. This paper presents a calibration procedure for cohesive bulk materials where the parameters for the Hybrid contact model are discussed in detail. A series of calibration simulations with systematic parameter variation is undertaken to define a set of calibration matrices. The developed calibration matrices enabled the formation of a parameter database, which can be used for the simulation of on-site applications to optimise plant geometry and other operational parameters.

1. Introduction

With the exploitation of ore bodies which would be typically disregarded and avoided, the materials handling sector must optimise their operations to handle problematic iron ores to keep up with current demands. Handling issues arise causing problems in all phases of the materials handling stream due to problematic iron ores and measures must be set in place to reduce downtimes of the materials handling sector. Problematic iron ores commonly have increased clay and moisture contents and may be found near or even below the water table. These ores are defined as Wet and Sticky Material (WSM) which cause handling issues in all areas of the materials handling stream from remains left in train wagons, the clogging of screens, to chute build-up, among others, which can cause the costly downtime of mining operations [1, 2]. The additional handling costs due to downtime and sub-optimal running conditions for systems with WSMs has been shown in the range of 4 to 6 AUD per tonne [3]. This would naturally be an area of concern financially for the mining industry and measures must be set in place to increase the likelihood of these systems performing effectively.

WSMs are problematic within the material handling stream due to the inter-particle and boundary cohesion and adhesion forces. In the field of bulk material handling, adhesion can be defined as the tensile force for particle-to-particle and particle-to-wall contact of the bulk material, whilst cohesion is the shear resistance for particle-to-particle and particle-to-wall contact under zero normal stress [4]. It has been further established that adhesion will only be of interest within bulk material handling for ores that also have cohesive characteristics [5]. These bulk materials that show both characteristics are able to cause blockages within a material handling system and are typically defined as a WSM. For the successful implementation of a WSM into the Discrete Element Method (DEM), new contact
models must be investigated. Currently DEM can accurately model dry free flowing materials such as gravels and other coarse granular materials. DEM does this by incorporating the rolling friction and wall friction coefficients into the well-defined Hertz contact model. However, as WSMs have higher moisture content, the contact mechanism becomes much more complex as the effect of surface tension between two particles, due to various bonding forces, starts to emerge [5]. These effects will not only apply additional bonding forces between the particles, but will also alter the frictional properties of the particles and walls, which in effect, changes the flow characteristics of the bulk material [6].

With the expansion of computation power, it is currently more feasible to use DEM for the contact models, typically referred to as cohesion models, required to describe the adhesion and cohesion mechanisms that will encapsulate the behavioural traits that WSMs show. Cohesion contact models will incorporate an additional force which will essentially ‘hold’ the particles together acting as the cohesion and/or adhesion which will be present. This additional force is incorporated to the contact models used to describe the particle rolling and sliding friction which governs the motion of the particle when subjected to an external force. This is undertaken in both the normal and tangential components for particle-to-particle and particle-to-wall contacts. There are numerous cohesion contact models available in several commercial and open source DEM packages. Each of the available cohesion contact models can be classified into three categories:

1. Elastic adhesive normal contact models.
2. Adhesive normal contact models including plasticity.
3. Capillary force (liquid bridging) contact models.

It is beyond the scope of this research and not feasible to discuss every contact model available in detail. It will be appropriate, however, to outline the cohesion contact model used for the simulations conducted in this research. The conducted simulations use the open source DEM software LIGGGHTS® [7] version 3.8.0 which has implemented cohesion contact models from each of the categories outlined above. To replicate the characteristics that WSMs show in practice, the coupling of two contact models has been proposed. The coupled contact model, referred to as the hybrid model, has produced the most realistic representation of a WSM. This is shown in the research of Carr et al., [8, 9]. The hybrid model is a combination of the Simplified Johnson-Kendall-Roberts (SJKR) model [10] for particle-to-wall contact and the Easo liquid bridging model [11] for particle-to-particle contacts. The coupled model has been found to be the most realistic model available from an industrial perspective where the solve times are acceptable for the accuracy of the obtained result. It will be appropriate to identify that the Edinburgh Elasto-Plastic Adhesion (EEPA) contact model [12] is capable of obtaining results which portray slightly more accurate results in comparison to the developed hybrid model. This however does come at the price of significantly longer computation times (estimated to be approximately eight times longer than the hybrid model). This will become much more evident when the quantity of particles in the simulation domain increases, such as the simulation of an industrial transfer chute which can operate up to 12,000 tonnes per hour for iron ore. Additionally, the vast array of parameters which require calibration for the EEPA model make the calibration procedure, significantly time consuming.

When the SJKR model is used for both particle-to-wall and particle-to-particle contacts, the resulting particle flow behaviour will result in a stiffer more rigid flow of the particles typically used to represent cohesive powders. Additionally, when the build-up of the bulk material onto a vertically mounted wall liner (representing the hood of a typical transfer chute) is considered, the SJKR fails to replicate these behaviours. Similarly, when the Easo liquid bridging model is used for both particle-to-wall and particle-to-particle contacts, the behaviours exhibited by WSMs are failed to be replicated when particle-to-wall contacts are considered. It is appropriate to identify, the characteristics of WSMs can be replicated using the Easo liquid bridging model for certain applications. This occurs for applications which only require particle-to-particle contacts to be considered. By coupling the SJKR model for particle-to-wall contact and the Easo liquid bridging model for particle-to-particle contact mechanism becomes much more complex as the effect of surface tension between two particles, due to various bonding forces, starts to emerge [5]. These effects will not only apply additional bonding forces between the particles, but will also alter the frictional properties of the particles and walls, which in effect, changes the flow characteristics of the bulk material [6].

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contact, a contact model capable of replicating the behaviours exhibited by WSMs for transfer system applications is created. This can be shown in the replication of the build-up of the bulk material onto a vertically mounted wall liner. A series of DEM calibration simulations with systematic parameter variation will be conducted to obtain the most accurate set of parameters to replicate the tested iron ore sample in the simulation domain. The developed calibration matrices allow for the formation of a parameter database, which can be used for the simulation of on-site applications to optimise plant geometry and other operational parameters. The explanation of the parameters which require systematic variation and the developed calibration procedure are outlined in the succeeding sections.

2. DEM Contact Model Input Parameters

Numerical modelling simulations require the calibration of parameters as an essential step for an accurate solution. This is especially found to be the case when DEM is considered. To replicate the behaviours a bulk material will show in reality, the sliding and rolling resistance of spherical particles must be considered. These parameters will ultimately influence the macroscopic behaviour of non-cohesive bulk materials [13]. By using spherical particles, a calibration procedure is necessary to replicate the behaviour of the bulk material. During the calibration procedure, the stiffness of the particles will typically dictate the required solve time [14, 15]. It is quite common to reduce the stiffness of the particles to improve the efficiency of the simulation solve time. This in effect makes the calibration of sliding and rolling resistance to be of critical importance. When the additional parameters required for the calibration of cohesive bulk materials are considered, the quantity of simulations and in effect time required for the calibration procedure to be undertaken significantly increases. It will therefore be essential to outline the parameters which require implementation into LIGGGHTS® [7] version 3.8.0 for the hybrid contact models (outlined above).

During the initial parameter input for the developed hybrid contact model, parameters are loaded into an input script which will call LIGGGHTS® [7] to run the simulation. The following parameters are required for implementation prior to the simulation:

- Surfacial liquid volume to solids volume, $V_{slc}$, defines the liquid volume surrounding the particles (measured moisture content is used).
- Surface tension, $\sigma_{ST}$, defines the surface tension of the liquid bridge acting between the particles.
- Fluid viscosity, $\mu_f$, defines the viscosity of the fluid in the liquid bridge acting between the particles (assumed to be water i.e. 0.00089 [Pa.s]).
- Contact angle, $\theta$, defines the angle of contact formed between the liquid bridge and the particles (assumed to be 60°).
- Adhesion energy density, $\Omega_{AED}$, defines the amount of adhesion which will be acting between the particles and the boundary surfaces (sticking the particles to surfaces).

In addition to the input parameters outlined above, the particle sliding friction and particle rolling friction are also required as input parameters. A systematic parameter variation approach has been utilised for the calibration procedure, outlined below, of the developed hybrid contact model. The parameters which require iteration as part of the calibration process for particle-to-particle contacts include the particle sliding friction, particle rolling friction and the surface tension of the liquid bridge. When particle-to-wall contacts are considered, the iteration of the adhesion energy density is required. The remaining parameters of the hybrid contact model are found to be non-sensitive to the particle behaviour in comparison to the parameters which do require calibration. The parameters which have been used for the simulations undertaken to replicate the behaviours of the tested iron ore sample are outlined in the following section.

3. DEM Contact Model Input Parameters

The successful selection of a unique parameter set capable of replicating a range of lab experiments will be dictated by the calibration procedure used. These lab experiments must consider a range of materials handling processes where different flow regimes are used in the aim to replicate industrial processes. For instance, typical lifting cylinder Angle of Repose (AOR) measurements will fail to
capture the dynamic flow conditions which may be experienced on site in an industrial transfer system. To address these potential drawbacks of DEM, it will be essential to calibrate problematic bulk materials with experimental measurements capable of providing flow regimes which can assist in replicating industrial processes. The developed calibration procedure uses a range of lab experiments which consider a range of flow regimes. Each of these experiments considers dynamic flow conditions in the aim of replicating problematic bulk material behaviours as they negotiate the materials handling stream.

One of the most debated topics in DEM is the consideration of the particle size range which is simulated. It will be unfeasible and almost impossible to undertake any simulation which will consider an industrial materials handling system if the real Particle Size Distribution (PSD) is considered. For instance, if a simple shear box calibration simulation (outlined in the following section) was undertaken using the real PSD, the quantity of particles is far beyond the current capabilities of modern-day computers. This is best explained if the tested iron ore sample was considered, where 40 kg of sample would be required to undertake an experimental measurement. In the case where the real PSD of the tested iron ore was used to conduct a simple shear box simulation, approximately 427 million particles would be required. This problem will become much more concerning if a transfer system which operates in excess of 12,000 tonnes per hour required a DEM simulation to be conducted. For these reasons, it will be necessary and more appropriate to use either a scalped or scaled PSD for the simulations conducted in this research. The calibration simulations have been undertaken using parameters to replicate the behaviours of the tested iron ore sample. A modified PSD will be required to undertake the simulations in a realistic timeframe. A scalped particle size will be utilised where the PSD curve is shown in Figure 1. A cut-off range has been set where any particles below this threshold will be assumed to be 5.6 mm. The particle size ranges above the set threshold use the same values as those which were measured in the lab.

![Figure 1 – Particle size distribution of iron ore sample showing scalped particle size range.](image)

The selection of input parameters requires careful consideration and, in most cases, experimental measurement values are used as input variables. In the case where measured values can be used, these will remain constant for all of the simulations undertaken within the scope of this research. For the values which cannot be directly measured with experimental measurements, the calibration of these parameters, using the developed calibration procedure, will be undertaken. A summary of the parameters which are required to undertake the simulations are shown in Table 1.
Table 1 – DEM Parameters for Iron Ore Sample

<table>
<thead>
<tr>
<th>Input Parameter</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time Step</td>
<td>[s/step]</td>
<td>9e-6</td>
</tr>
<tr>
<td>Coefficient of Restitution</td>
<td>[-]</td>
<td>0.3</td>
</tr>
<tr>
<td>Bulk Density</td>
<td>[kg/m³]</td>
<td>1400</td>
</tr>
<tr>
<td>Particle Density</td>
<td>[kg/m³]</td>
<td>increased depending on Surface Tension</td>
</tr>
<tr>
<td>Poisson’s Ratio</td>
<td>[-]</td>
<td>0.3</td>
</tr>
<tr>
<td>Young’s Modulus</td>
<td>[Pa]</td>
<td>1e8</td>
</tr>
<tr>
<td>Particle Sliding Friction</td>
<td>[-]</td>
<td>see Table 2</td>
</tr>
<tr>
<td>Particle Rolling Friction</td>
<td>[-]</td>
<td>see Table 2</td>
</tr>
<tr>
<td>Wall Friction (Perspex)</td>
<td>[-]</td>
<td>0.32</td>
</tr>
<tr>
<td>Wall Friction (Rubber Belt)</td>
<td>[-]</td>
<td>0.55</td>
</tr>
<tr>
<td>Wall Friction (Ceramic Wall Liner)</td>
<td>[-]</td>
<td>0.68</td>
</tr>
<tr>
<td>Wall Friction (Mild Steel Wall Liner)</td>
<td>[-]</td>
<td>0.65</td>
</tr>
<tr>
<td>Adhesion Energy Density (AED)</td>
<td>[J/m³]</td>
<td>see calibration procedure section</td>
</tr>
<tr>
<td>Surficial Liquid Volume</td>
<td>[%]</td>
<td>18.5</td>
</tr>
<tr>
<td>Surface Tension (ST)</td>
<td>[N/m]</td>
<td>see Table 2</td>
</tr>
<tr>
<td>Fluid Viscosity</td>
<td>[Pa.s]</td>
<td>8.9e-4</td>
</tr>
<tr>
<td>Contact Angle</td>
<td>[°]</td>
<td>60</td>
</tr>
</tbody>
</table>

The determination of the wall friction coefficients and bulk density measurements used for the simulations conducted in this research have been undertaken using the procedures outlined in AS3880 [16]. The time step and Young’s Modulus of the particles have been set to values which are sufficient to run the simulations in a reasonable timeframe. Additionally, these values produce results where the particles in the simulation domain are stable. This is best explained when the particles of the shear box test (outlined in the proceeding section) are considered, where the resulting mass of particles will remain stable once the box has been filled. In the case where a lower Young’s Modulus value is used, a pulsing velocity field can be observed. This is attributed to the spherical particles being too soft and the dissipation of energy in the system requiring significantly longer times to achieve steady state. It will be appropriate to identify the density of the particles require to be adjusted depending on the calibrated parameters. This is best explained if a simple shear box test (outlined in the proceeding section) is considered. For this case a higher number of particles are required to fill the same volume if a lower surface tension (amount of cohesion) is compared to using higher values of surface tension. Due to the dynamic flow regimes of the calibration experiments, it is essential to match the bulk density between experimental measurements and simulation results.

4. DEM Calibration of Wet and Sticky Bulk Materials
Calibration procedures for dry non-cohesive bulk materials exist which typically alter the simulation parameters using a systematic variation of parameter approach [13, 17]. To determine the friction parameters for dry non-cohesive bulk materials there are many calibration experiments which exist. Some of the notable calibration experiments include; the Angle of Repose (AOR) experiment [13, 18], shear box experiment [8, 19] and more recently the draw down experiment [20, 21]. General calibration procedures will typically use a single experiment to determine the sliding and rolling friction parameters for dry non-cohesive bulk materials. This results in a multitude of parameter combinations which can replicate the experiment which is being simulated. By only using a single
calibration experiment, the selection of a unique parameter combination is extremely difficult to obtain [13]. In the work of Roessler et al. [20], a procedure for the calibration of non-cohesive bulk materials using a range of calibration experiments is considered. This enabled for the use of several calibration experiments to be conducted which would then result in several reference values for the calibration. An alternative to several experiments would be one calibration test which allows the measurement of several results as calibration criteria. This in turn will result in a unique parameter combination. With the determination and correct use of unique parameter settings, users of DEM can have confidence that the selected parameter settings will be capable of replicating any materials handling system. When the calibration of WSMs is considered, new calibration methods must be utilised. This is due to the additional adhesion parameters which are required for use in the more complex contact models. These additional parameter settings also require calibration in addition to the sliding and rolling resistance. This in turn significantly increases the quantity of simulations and time required for a typical calibration. To undertake the calibration of WSMs using a systematic parameter variation approach, a new method is proposed. To ensure a unique parameter set is obtained, sufficient calibration experiments are essential. The calibration experiments used for the determination of a unique parameter set of the tested iron ore sample are outlined in the following section.

4.1 Calibration Experiments
The calibration of parameters is key to the accuracy of any DEM simulation. When determined correctly, the selected parameter set can represent the physical behaviours which a bulk material will show in practice. It is therefore necessary to undertake experiments to calibrate the parameters identified in Table 1. For the DEM simulations conducted within this research, a range of calibration experiments have been undertaken on an iron ore sample at 18.5% MC. These calibration experiments are undertaken in two streams for particle-to-particle and particle-to-wall contacts. When the more complex particle-to-particle contacts are considered, two calibration experiments have been used. These include shear box tests and draw down tests, where the arching case of the draw down testing will be used for validation of the particle-to-particle calibration. For the particle-to-wall contact calibration, the dynamic adhesion inclined plate test (represents the spoon of a transfer chute) is utilised. Shear box experiments, typically referred to as slump tests, are used to identify the internal strength of a bulk material when no consolidation loads are applied. A schematic of the shear box testing apparatus is shown in Figure 2 and will represent a dynamic calibration scenario. The shear box used is constructed from Perspex and has a length, width and height of 300 mm. One of the vertical walls is removable to allow the bulk material to flow (slump) out of the shear box.

![Figure 2 – Schematic of shear box testing apparatus.](image)

To replicate the discharge of a hopper or bin, the draw down test has been developed. The draw down test, as shown in Figure 3, consists of an upper and lower box where each box is 500mm high, 500mm wide and 100mm deep. The upper box has a discharge gate (flaps) and an adjustable rectangular opening at the bottom. The discharge gate is rapidly opened (0.3 seconds) and the bulk material sample is allowed to discharge into the lower box. The outflowing bulk material forms a stock pile in
the lower box (AOR measurement), while the remaining bulk material forms two slopes in the upper box (shear angle measurement).

Figure 3 – Schematic of draw down testing apparatus.

To replicate the dynamic flow conditions of a bulk material onto the spoon of a transfer chute, the dynamic adhesion inclined plate test has been undertaken. This calibration test consists of a 450 mm wide belt conveyor situated 1500 mm above a wall liner which allows for varying angles to be investigated. By investigating a range of wall liner angles, the threshold adhesion present in a bulk material sample for particle-to-wall contacts can be determined. A schematic of the dynamic adhesion inclined plate test is shown in Figure 4. The residual mass and maximum build-up height perpendicular to the wall liner surface are determined for a range of wall liner angles. The upper (no residual mass) and the lower (highest residual mass) tested wall liner angles are used for the DEM calibration of the Adhesion Energy Density (AED).

Figure 4 – Schematic of dynamic adhesion inclined plate testing apparatus.
4.2 Calibration Procedure and Flow Chart

The calibration of WSMs can be extremely complex depending on the modelling application which is required to be simulated. This is attributed to the additional adhesion parameters which are required for use in the more complex contact models. To reduce this complexity, the developed calibration procedure considers two calibration streams which will be undertaken for particle-to-particle and particle-to-wall contacts separately. Due to the vast array of parameters required to calibrate for particle-to-particle contacts, it will be appropriate to calibrate these parameters first. The proposed calibration procedure flowchart for particle-to-particle contact is shown in Figure 5. The calibration experiments required for particle-to-particle calibration of a WSM include shear box testing and draw down testing. The first stage of the particle-to-particle calibration will use the shear box experiment. Once the residual mass and shear angle are determined from the shear box experimental measurements, the minimum and maximum surface tension limits are required. The minimum limit is determined when the mass in the shear box for a particle sliding friction and rolling friction of 0.9 results in a lower value than the experimental value. The maximum limit is determined when all of the particles remain in the shear box for a particle sliding friction and rolling friction of 0.3.

Figure 5 – Calibration procedure for particle-to-particle contacts.
After the surface tension limits are determined, the systematic parameter variation process will begin. This is undertaken by iterating the particle sliding friction, rolling friction and surface tension. The iteration values used for the shear box calibration of the tested iron ore sample are shown in Table 2. The remaining input variables which have been used for the simulations conducted in this research are outlined in Table 1. It will be appropriate to identify when the surface tension of the liquid bridge acting between the particles increases, the bulk density of the sample will also increase. This is best explained in reference to the shear box overfilling when compared to the same particle values without additional cohesion. To incorporate this effect into the calibration procedure, the density of the particles in the simulation are adjusted so the volume and mass within the shear box remains constant.

<table>
<thead>
<tr>
<th>Contact Model Parameter</th>
<th>Units</th>
<th>Parameter Iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle Sliding Friction</td>
<td>[-]</td>
<td>0.3 : 0.1 : 0.9</td>
</tr>
<tr>
<td>Particle Rolling Friction</td>
<td>[-]</td>
<td>0.3 : 0.1 : 0.9</td>
</tr>
<tr>
<td>Surface Tension</td>
<td>[N/m]</td>
<td>1.0 : 0.5 : 3.5</td>
</tr>
</tbody>
</table>

Once the shear box simulations have been completed, a reduction of parameter sets occurs by applying thresholds for the remaining mass and the measured shear angle, $\varepsilon_S$, which are determined from the experimental measurements. The threshold values which have been used for the DEM calibration of the tested iron ore sample were set to ±5%. After the reduction of parameters sets has been conducted, the remaining parameter sets are reduced further by simulating the draw down testing apparatus for a flowing case. Upon completion of the draw down calibration simulations, the final reduction of parameter sets occurs by applying thresholds for the remaining mass, the measured shear angle, $\varepsilon_D$, and the measured AOR, $\omega_D$, which are determined from the experimental measurements. To validate the remaining parameters sets and select a unique parameter set, the draw down testing apparatus is simulated for an arching (blockage) case. The resulting simulations are compared to the measured remaining mass, which is determined from the experimental measurements. A summary of the obtained calibration simulation results are outlined in the following section.

After a unique parameter set has been selected for the particle-to-particle contacts using the procedure outlined in Figure 5, it will be appropriate to calibrate the particle-to-wall contacts using the procedure outlined in Figure 6. The calibration experiments required for particle-to-wall calibration of a WSM include the dynamic adhesion inclined plate test. The first stage of the particle-to-wall calibration will require the residual mass for each of the tested wall liner angles, $\beta_{wall}$, to be determined from the dynamic adhesion inclined plate experimental measurements. Once these residual mass values are determined, the minimum and maximum Adhesion Energy Density (AED) thresholds are required. The minimum limit is determined when the particles begin to stick on the wall liner for shallowest tested angle. The maximum limit is determined when particles begin to stick on the wall liner for steepest tested angle. The maximum and minimum adhesion energy density limits for the tested iron ore sample occurred when the AED was $15e^5$ J/m$^3$ and $4e^5$ J/m$^3$ respectively. After the AED limits are determined, the systematic parameter variation process for particle-to-wall contacts will begin by iterating the AED between the determined limit values. This will be conducted for the unique particle-to-particle parameter setting.
Once the dynamic adhesion inclined plate simulations have been completed, a reduction of the AED parameter set occurs by applying a threshold for the residual mass on the selected (shallowest) wall liner. These residual mass values are determined from the experimental measurements. The threshold values which have been used for the DEM calibration of the tested iron ore sample were set to ±10%. A summary of the obtained calibration simulation results are outlined in the following section. To validate the selected parameter set, a further simulation will be conducted using a different wall liner angle.

5. Calibration Simulations

To identify if a unique parameter setting can be selected, a series of calibration simulations are undertaken using the developed calibration procedure. These calibration simulations will be conducted for the parameters outlined in Table 1. The first stage of the calibration simulations will require the limits for the amount of surface tension (cohesion) to be identified. This is undertaken using the shear box test where the limits and corresponding iteration (calibration) values are shown in Table 2. A total of 294 (7 x 7 x 6) simulations are required to undertake the first stage of the calibration procedure. Once the initial calibration simulations are undertaken, a reduction of parameter sets can occur. The residual mass and the measured shear angle, $\varepsilon_S$, which are determined from the experimental measurements are utilised to reduce the parameter sets from the initial shear box simulations. The threshold values which have been used for the DEM calibration of the tested iron ore sample were set to ±5%. It will be appropriate to identify that the following section will show
the results of the selected (unique) parameter settings only where it has been deemed unnecessary to show all the potential parameters sets which remained once the thresholds identified above had been implemented. The selected parameter setting which will be used for the reminder of the simulations conducted within this research are shown in Table 3.

Table 3 – Hybrid Contact Model Calibrated Parameter Values

<table>
<thead>
<tr>
<th>Contact Model Parameter</th>
<th>Units</th>
<th>Parameter Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle Sliding Friction</td>
<td>[-]</td>
<td>0.5</td>
</tr>
<tr>
<td>Particle Rolling Friction</td>
<td>[-]</td>
<td>0.3</td>
</tr>
<tr>
<td>Surface Tension</td>
<td>[N/m]</td>
<td>3.5</td>
</tr>
</tbody>
</table>

The comparison between shear box experimental measurements and simulated data for the selected parameter set is shown in Figure 7, where the similarities of the measured shear angle can be immediately identified. This becomes evident when the residual mass and measured shear angle are considered.

![Figure 7](image1.png)

Figure 7 – Comparison between experimental and simulation result for shear box testing.

A summary of the comparison to simulated data and experimental measurement values for the shear box test are shown in Table 4. It will be appropriate to identify that the residual mass is a more definitive threshold in comparison to the measured shear angle. This is attributed to the erroneous measurements of the shear angle which can vary by up to 5° depending on the interpretation of where the angle should be measured.

Table 4 – Shear Box Testing Results Comparison

<table>
<thead>
<tr>
<th>Reference</th>
<th>Units</th>
<th>Experimental</th>
<th>Simulation</th>
<th>Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Residual Mass</td>
<td>[kg]</td>
<td>30.8</td>
<td>30.2</td>
<td>-2.0 %</td>
</tr>
<tr>
<td>Shear Angle</td>
<td>[°]</td>
<td>65.5</td>
<td>67.2</td>
<td>+2.5 %</td>
</tr>
</tbody>
</table>

The second stage of the calibration process will utilise the draw down test for a flowing case and can occur once the reduction of parameter sets has been undertaken. The comparison between draw down experimental measurements and simulated data for the selected parameter set is shown in Figure 8, where the similarities of the measured shear angle and AOR can be immediately identified. This becomes evident when the residual mass, measured shear angle and measured AOR are considered.
A summary of the comparison to simulated data and experimental measurement values for the flowing case of the draw down test are shown in Table 5. Similar to the shear box test, it will be appropriate to identify that the residual mass is a more definitive threshold in comparison to the measured shear angle and measured AOR. This is attributed to the erroneous measurements of the shear angle and AOR which can vary by up to 5° depending on the interpretation of where the angle should be measured.

The final stage of the particle-to-particle calibration process will utilise the draw down test for an arching (blockage) case. This can occur once the draw down simulations for a flowing case using the reduced parameter sets has been undertaken. The comparison between draw down experimental measurements and simulated data for the selected parameter set is shown in Figure 9, where the visual similarities are shown. Since the validation of particle-to-particle calibration utilises an arching (blockage) case, measurements of the shear angle and AOR cannot be undertaken. It is therefore more appropriate to consider the residual mass which is used for the comparison between experimental measurements and simulated data. The residual mass of the simulation was found to be 1.86 kg which resulted in a deviation of -5.4% from the experimental measurement.
The calibration of particle-to-wall contacts will utilise the calibration procedure outlined in Figure 6. The first stage will be to determine the thresholds for the AED which was determined to range between $15e^5$ J/m$^3$ and $4e^5$ J/m$^3$. Once these values are determined, the calibration of particle-to-wall contacts can be undertaken using the dynamic adhesion inclined plate testing apparatus for a build-up case. It will be appropriate to identify, the selected parameter set for particle-to-particle contacts, as determined above, will also be utilised. The comparison between dynamic adhesion inclined plate experimental measurements and simulated data for the selected parameter set (AED $12e^5$ J/m$^3$) is shown in Figure 10, where the visual similarities of the residual build-up can be identified. This becomes evident when the residual mass, is considered. The residual mass of the simulation was found to be 14.72 kg which resulted in a deviation of -7.9% from the experimental measurement.
Once the calibration of particle-to-wall contacts has been undertaken using the dynamic adhesion inclined plate testing apparatus for a build-up case, a different wall liner angle (no build-up) is considered to validate the chosen AED value. Similar to the build-up case of the dynamic adhesion inclined plate simulations, the selected parameter set for particle-to-particle contacts, as determined above, will also be utilised. The comparison between dynamic adhesion inclined plate experimental measurements and simulated data for the selected parameter set (AED $12e^5$ J/m$^3$) is shown in Figure 11, where the visual similarities of no residual build-up are shown. This becomes evident when the residual mass, is considered. The residual mass of the simulation was found to be 0.41 kg which resulted in a deviation of -9.8% from the experimental measurement.

For the simulation of WSMs, the developed hybrid contact model has been observed to be a more efficient and better representation of industrial applications, as shown above. This becomes evident when the parameter set (which requires iteration) and the computational solve times are considered. This can be best determined when the comparison between the hybrid contact model and EEPA contact model are considered. The EEPA model was able to replicate the behaviours of bulk material blockages within transfer chute systems to some degree. However, when the computational solve times and the vast array of parameters are considered, this model was deemed to be unpractical for use in industrial cases.

6. Conclusions

This paper has presented a calibration methodology to model the blockages of transfer chute systems typically caused by WSMs. The coupling of the SJKR and Easo Liquid Bridging models, referred to as the hybrid model, is proposed and consequently used to predict problematic bulk material behaviour. A calibration procedure has been developed and undertaken where the parameters for each cohesion model were discussed. A series of calibration simulations with systematic parameter variation were undertaken to define a set of calibration matrices where a unique parameter setting was identified. By using a systematic parameter variation approach, a method is developed which can be utilised as proof for the more recent optimisation algorithms which are currently used for the calibration of non-cohesive materials. Furthermore, the developed calibration matrices enabled the formation of a parameter database, which can be used for the simulation of on-site applications to optimise plant geometry and other operational parameters.
References


