Effect of Particle properties on the Discrete Element Simulation of Wall Friction

Andrew Grima  
*University of Wollongong*, agrima@uow.edu.au

Peter Wypych  
*University of Wollongong*, wypych@uow.edu.au

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Keywords
particle, properties, discrete, element, simulation, effect, wall, friction

Disciplines
Engineering | Science and Technology Studies

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Effect of Particle properties on the Discrete Element Simulation of Wall Friction

Andrew Grima and Peter Wypych

Faculty of Engineering and Information Sciences
University of Wollongong, Northfields Avenue, Wollongong NSW 2522
agrima@uow.edu.au

Abstract

Modelling the interaction between particles and boundaries is of great interest and importance in many Discrete Element Method (DEM) applications where boundary failure conditions dictate the flow behaviour and velocity gradients of a bulk material. Bulk wall friction angles in DEM models are dependent on the mechanical properties of the particles and boundary material as well as the constraints of the contact models used, especially the tangential and rolling torque components. This paper examines the parameters determined from the calibration inclination test by conducting direct wall shear tests to validate the accuracy of the calibration parameters and the sensitivity of particle-to-boundary parameters of the material model using the Hertz-Mindlin (H-M) and H-M with linear cohesion contact models. The influence particle geometry has on wall friction is also examined where results from the DEM simulations are compared against the corresponding results from a large-scale shear tester. The 3-sphere cluster particle developed in this study is found to provide the most representative bulk shear behaviour where the wall yield loci predicted by DEM agree well with all experimental results.

1. Introduction

The interaction of a granular material with boundary materials is one of the most important factors to consider when designing and modelling mass flow hoppers, chutes, feeders and other equipment where flow is expected to occur. Proper calibration of the relationship between the normal wall stress and shear stress is required to obtain reliable DEM predictions for design and trouble-shooting application. Bulk wall friction angles in DEM models are dependent on the mechanical properties of the particles and boundary material as well as the constraints of the contact models used, especially the tangential and rolling torque components.

Grima and Wypych [1] described a simple and quick inclination test to assist in the calibration of a DEM material model for a dry and cohesionless bulk material, polyethylene pellets. Further research has examined the parameters determined from the inclination test by conducting direct wall shear tests on dry and wet bauxite to validate the accuracy of the inclination calibration technique and the sensitivity of particle-to-boundary parameters of the material model using the H-M [2] and H-M with linear cohesion [3] contact models. The (more challenging) cohesive bauxite results and findings are presented in this paper. The influence particle geometry has on wall friction is also examined where results from the DEM simulations are compared against the corresponding results from a Large-Scale Wall Friction Tester, (LSWFT) developed by Grima et al [4].
2. Experimental Work

The authors were requested to model and study the flow of bauxite under variable moisture conditions through an industrial-scale conveyor transfer chute lined with Bisplate 400. Wall friction tests were undertaken on a sample of bauxite under dry and maximum strength moisture conditions (viz. 0 and 11% wet basis, respectively). A sample of the chute liner material was obtained for this study and installed on the LSWFT, where the LSWFT is shown in Figure 1.

![Figure 1: Large-Scale Wall Friction Tester (LSWFT)](image)

The LSWFT was selected instead of the Jenike Direct Shear Tester (JDST), because of the following reasons:
1. The JDST uses a shear cell with an internal diameter of 95.25 mm and is generally limited to the testing of sub 4 mm bulk material samples.
2. The shear rate of the original JDST is only 2.69 mm min\(^{-1}\) [5]
3. Items (1) and (2) are quite acceptable for “quasi-static” applications, such as bin and hopper design, but are inadequate for “dynamic” applications, such as high-speed conveyor transfers.
4. Also, handling and preparing a moist product for wall friction testing according to the standard shear testing technique [5] can easily change the characteristics of the product by drying, sieving and wetting the product.
5. The LSWFT provides the capability to measure “as received” products with a wider particle size distribution (e.g. top size of approximately 30 mm) without having to spend a great deal of time drying (if required), sieving the product and readjusting the moisture content to the correct conditions. It also can be operated at much higher shear rates than the JDST. This is important for “dynamic” (kinetic friction) applications, where the coarse fraction of the material can also have a significant impact on flow behaviour.

The cohesive bauxite wall friction results are presented later in this paper, where comparisons are made directly with the DEM simulations.

3. DEM Parameters

Wall friction simulations were conducted initially using the H-M model for the particle-to-particle and particle-to-boundary contacts to model the dry (cohesionless) bauxite. The H-M with linear cohesion model was then used to model cohesive bauxite at maximum strength conditions. Table 1 lists the various parameters for the bauxite particles and Bisplate 400 that were implemented into
the DEM models. Note: most of the parameters given in Table 1 are based on direct measurements, but some are approximations based on other sources, which are referenced accordingly.

To investigate the influence of particle geometry and the moment of inertia on wall friction angles of an assembly of particles, three different particle geometries of relevant size distribution (referred to as Particle A, B and C), as indicated in Figure 2, were used to model the bauxite. The non-spherical particles were created by clustering spheres together to represent non-spherical particles as discussed by Favier et al [6]. The aim of using three particle shapes was to examine the variation in the bulk behaviour of the assembly of particles using the different shaped discrete elements to model the bauxite as a bulk sample. To realistically model particle rotational motion and account for non-spherical characteristics of real materials that can’t be easily modelled such as surface asperities, sharp edges, flat surfaces and structure, a rolling resistance model is also included. A Type A directional constant torque model as categorised by Ai [7] was implemented to oppose the relative rotation between particles and between particles and wall surface.

The time step, $\Delta t$, used in DEM simulations (using explicit time integration) is important to maintain numerical stability. This paper investigates the influence of the time step on wall friction where $\Delta t$ has been selected based on a ratio of the Rayleigh time step, $t_r$, shown by Kremmer and Favier [8]. When using Hertz-based contact models, $t_r$ is calculated based on the critical frequency for Rayleigh waves to propagate across the surface of a particle.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_{s,p}$</td>
<td>2300</td>
<td>kg m$^{-3}$</td>
<td>Bauxite, measured using a pycnometer</td>
</tr>
<tr>
<td>$\rho_{s,w}$</td>
<td>7630</td>
<td>kg m$^{-3}$</td>
<td>Bisplate 400, measured</td>
</tr>
<tr>
<td>$E_p$</td>
<td>171.6</td>
<td>MPa</td>
<td>Bauxite, approximated using a Ultra-Micro-Indentation System</td>
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<tr>
<td>$E_w$</td>
<td>207</td>
<td>GPa</td>
<td>Bisplate 400, approximated from Callister [9]</td>
</tr>
<tr>
<td>$\nu_p$</td>
<td>0.3</td>
<td>-</td>
<td>Bauxite, approximated from Gercek [10]</td>
</tr>
<tr>
<td>$\nu_w$</td>
<td>0.3</td>
<td>-</td>
<td>Bisplate 400, approximated from Callister [9]</td>
</tr>
<tr>
<td>$\mu_{s,p,p}$</td>
<td>0.78</td>
<td>-</td>
<td>Bauxite-to-Bauxite, measured using a static inclination test shown by Grima and Wypych [1]</td>
</tr>
<tr>
<td>$\mu_{s,p,w}$</td>
<td>0.48</td>
<td>-</td>
<td>Bauxite-to-Bisplate 400, measured using a static inclination test shown by Grima and Wypych [1]</td>
</tr>
<tr>
<td>$e_{p,p}$</td>
<td>0.4</td>
<td>-</td>
<td>Bauxite-to-Bauxite, measured using a high speed camera</td>
</tr>
<tr>
<td>$e_{p,w}$</td>
<td>0.54</td>
<td>-</td>
<td>Bauxite-to-Bisplate 400, measured using a high speed camera</td>
</tr>
</tbody>
</table>

Figure 2: Particle Shape Representations of Bauxite for Wall Friction DEM Models: (a) Particle A; (b) Particle B; and (c) Particle C
4. Wall Friction Models and Tests

Based on the standard shear testing technique [5], numerical wall friction tests were conducted as follows:
1. Particles were placed into the shear cell (see Figure 3) where a retainer (not shown in Figure 3) was used to retain excess particles.
2. Excessive particles were removed from the simulation domain by adjusting the domain boundaries but a small layer of particles above the top of the ring was left to allow for compaction of the particles.
3. The particle assembly was consolidated by lowering the cover to the top of the particles where a normal consolidation force $F_n$ was applied to the shear cell using a custom servo mechanism in EDEM [11].
4. The cover was twisted for approximately 3 seconds using sinusoidal rotation (rotation = 22 degrees, frequency = 3 Hz) to consolidate the particles as depicted in Figure 3 while subject to $F_n$. Upon completion of the consolidation, there were approximately 28500, 19800 and 18500 particles in the shear cell of Particle A, B and C, respectively.
5. Once the particles were consolidated, $F_n$ was reduced to the initial $F_n$ for shearing and the shear velocity of the Bisplate 400 was set. Similar to the LSWFT design, the shear cell remained stationary while the Bisplate 400 (modelled using a flat plane) was sheared under the shear cell. Note: wall friction tests are conducted on the JDST where the shear cell is sheared on top of a stationary wall sample.
6. When steady-state shear was achieved, $F_n$ was reduced and shearing continued until the lowest $F_n$ was obtained.
7. Four normal pressures of 10, 5, 2.5 and 0.5 kPa were applied to the cover.
8. Generally, the initial shear point is ignored when analysing the Wall Yield Locus (WYL) in a laboratory but due to the limitation of the number of simulations conducted, it was included.

Shear rates greater than the JDST value of 2.69 mm min$^{-1}$ occur in many bulk material handling applications and validating wall friction angles at greater shear rates is more relevant to accurately calibrate the DEM (dynamic) models. Shear rates of $V_s = 0.005$ m s$^{-1}$ (300 mm min$^{-1}$) and 0.05 m s$^{-1}$ (3000 mm min$^{-1}$) were selected for this investigation.

![Figure 3: Pre-Consolidation of Bauxite Particles in Shear Cell](image)

5. Experimental Results

Modelling the cohesion and adhesion between a bulk material and wall surface is of great interest in many applications to ensure that reliable flow occurs. It is rare that bauxite is handled in a completely cohesionless condition resulting in a degree of cohesion when water is added. The H-M with linear cohesion was used to model the cohesion between the particles and Bisplate 400 where the DEM results were compared against the WYL measured on the LSWFT with the bauxite at moisture content of 11% wet basis. The effects of cohesion between the particles and the ring and
cover have been neglected but the cohesion between the particles was considered in this investigation. The magnitudes of cohesion energy density, $C_{e \ p.w}$, required for the DEM models using Particles A, B and C were selected based on the results obtained from the simulations of moist bauxite and the inclination tests (where slippage occurred between 44 and 50 degrees): $C_{e \ p.w} = 7 \times 10^5$, $8 \times 10^5$ and $8 \times 10^5$ J m$^{-3}$ for Particle A, B and C, respectively. To examine the sensitivity of $C_{e \ p.w}$, a value 1.5 times greater than these suggested values was also used in the DEM models with Particles A and B. For Particle C, the wall friction was examined with values of $C_{e \ p.w}$ at $2 \times 10^5$, $4 \times 10^5$ and $6 \times 10^5$ J m$^{-3}$.

Figures 4 and 5 show the wall yield loci from the DEM simulations of the wall friction test where $V_s = 0.05$ and $0.005$ m s$^{-1}$ respectively, using the linear cohesion contact model and Particle A. Figure 4 indicates that the linear cohesion added into the DEM models results in minimal increase of the shear stress between the particles and wall sample where the WYL from the cohesionless (dry bauxite tests ($C_{e \ p.w} = 0$ J m$^{-3}$) has been included on Figure 4 to provide a comparison. When $C_{e \ p.w}$ is increased to $1.05 \times 10^6$ J m$^{-3}$, a good correlation between the experimental WYL and shear point at $\sigma_w \approx 4$ kPa occurs. However, when $V_s = 0.005$ m s$^{-1}$ a difference is noted when the linear cohesion model is incorporated into the DEM model, as an increase of the shear stress is observed in Figure 5 when $C_{e \ p.w}$ is increased. The error between the experimental and DEM WYL is low when $C_{e \ p.w} = 1.05 \times 10^6$ J m$^{-3}$, which is much greater than the value determined from the inclination test using Particle A. Figure 4 and 5 once again shows $\Delta t$ has a great influence on the WYL and shearing process, where a large $\Delta t$ produces poor results but $\Delta t \leq 0.3 t_r$ (when $t_r$ is calculated based on the minimum particle radius) seems to be adequate to obtain reliable and consistent results.

![Figure 4: Comparison of WYL using H-M with Linear Cohesion Contact Model (Particle A, $V_s = 0.05$ m s$^{-1}$, $\mu_{r \ p.w} = 0.25$, $\mu_{s \ p.w} = 0.48$)](image-url)
When Particle B is used to model the cohesive bauxite with $C_{e\,p.w} = 8 \times 10^5$ J m$^{-3}$, there is an improved correlation between the experimental and DEM wall yield loci shown in Figures 6 and 7, compared to the results when Particle A is used. When $\Delta t \approx 0.3t_r$, there is an increase of the shear stress when $C_{e\,p.w}$ is increased irrespective of $V_s$. When $C_{e\,p.w} = 1.2 \times 10^6$ J m$^{-3}$, there is an over-prediction of the shear stress at $\sigma_w \approx 4$ and 6 kPa when $V_s = 0.05$ m s$^{-1}$ but at a lower $V_s = 0.005$ m s$^{-1}$, the errors between the experimental and DEM results are minor. Reviewing Figures 6 and 7 indicates that $C_{e\,p.w} = 8 \times 10^5$ J m$^{-3}$ determined from the inclination calibration test is sufficient to model the increased cohesion between the bauxite particles close to maximum strength conditions and Bisplate 400, especially when $V_s = 0.05$ m s$^{-1}$.
Figure 7: Comparison of WYL using H-M with Linear Cohesion Contact Model (Particle B, $V_s = 0.005 \text{ m s}^{-1}, \mu_{r \text{ p.w}} = 0.2, \mu_{s \text{ p.w}} = 0.48$)

Figure 8 shows that the cohesion between the bauxite particles and Bisplate 400 can be modelled adequately using the H-M with linear cohesion model with Particle C. In fact, Particle C obtains good linear wall yield loci, which are dependent on $C_{e \text{ p.w}}$. Figure 8 indicates that $C_{e \text{ p.w}} = 2 \times 10^5$ J m$^{-3}$ is more than adequate to obtain a good correlation between the experimental and DEM wall yield loci when $V_s = 0.05$ and 0.005 m s$^{-1}$. Under confined conditions, such as the wall friction test, the required $C_{e \text{ p.w}}$ is much lower than the estimated value determined from the inclination calibration method where the contact forces are of lower magnitude compared to the wall shear test. When using Particle C, greater particle interlocking occurs, restraining the rotational behaviour of the particles compared to Particles A and B. The coefficient of rolling friction used with Particle C was also reduced from 0.25 and 0.2 used for Particle A and B respectively to 0.01. As the particles cannot rotate as easily, greater sliding occurs between the particles and boundary, making the linear cohesion model more sensitive to $C_{e \text{ p.w}}$ under confined conditions. Under rapid flow conditions, such as chute flow, where the coordination number is low and particles can rotate with more freedom, a conservative $C_{e \text{ p.w}}$, determined from the inclination calibration test, is still plausible but is too high for compacted bed applications such as discharge from a silo where the wall pressures are much greater.

Figure 8: Comparison of WYL using H-M with Linear Cohesion Contact Model (Particle C, $\mu_{r \text{ p.w}} = 0.01, \mu_{s \text{ p.w}} = 0.48, \Delta t = 32.5 \mu s$)
6. Discussion and Conclusions

Numerical validations of direct wall shear tests have been conducted to examine the normal wall and shear stress relationship using the H-M and H-M with linear cohesion models to simulate the shearing of dry and moist bauxite against rough Bisplate 400. Due to particle scale-up, there was a limitation of the minimum normal wall stress that could be investigated. As there are no physical limitations of inverting the shear cell in a DEM model by changing the vector of the gravitational acceleration or assigning a very low solids density to the particles, there is scope for future investigations to verify the cohesion of the particle assembly at low normal stress using scaled particle size distribution.

This study has shown that appropriate selection and calibration of DEM parameters can achieve satisfactory, if not perfect bulk behaviour of the bauxite shearing against a boundary surface. The important observations and conclusions arising from this investigation are:

- Based on the rolling friction model and rolling friction constraints (e.g. coefficient of rolling and static friction, maximum angular velocity) investigated in this paper, spherical particles were observed to roll too much (rather than slide) during shear tests.
- The rolling torque model used is not sufficient to restrain rotation of the spherical particles.
- Modelling the particles with a greater degree of blockiness and non-sphericity provides a better correlation between the experimental and DEM results as particle rotation is mechanically restrained and does not rely on rolling torque models to restrict rotation.
- Particle C obtained the best bulk shear behaviour where the DEM wall yield loci matched the experimental data well when modelling the bauxite under cohesive conditions.
- The numerical time step is important during the confined shearing of particles as strain rate and tangential velocity is critical to obtain reliable results from the contact models.
- The approximation of $\mu_{s,p,w}$ from the LSWFT and $C_{e,p,w}$ from the LSWFT and inclination test seem sufficient to develop a rough DEM material model for the particle-to-boundary interactions without having to conduct time consuming wall shear tests. However when particles with a high blockiness factor are utilised to characterise a bulk material, care is required when selecting $C_{e,p,w}$ to model a cohesive product subject to high consolidation pressures.

7. Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>$C_e$</td>
<td>Cohesion energy density for linear cohesion model, J m$^{-3}$</td>
</tr>
<tr>
<td>$e$</td>
<td>Coefficient of restitution</td>
</tr>
<tr>
<td>$E$</td>
<td>Young's modulus of elasticity, Pa</td>
</tr>
<tr>
<td>$F_n$</td>
<td>Normal force, N</td>
</tr>
<tr>
<td>H-M</td>
<td>Hertz-Mindlin</td>
</tr>
<tr>
<td>JDST</td>
<td>Jenike Direct Shear Tester</td>
</tr>
<tr>
<td>LSWFT</td>
<td>Large-Scale Wall Friction Tester</td>
</tr>
<tr>
<td>$t_r$</td>
<td>Rayleigh time step, s</td>
</tr>
<tr>
<td>$V_s$</td>
<td>Shear rate, m s$^{-1}$</td>
</tr>
<tr>
<td>WYL</td>
<td>Wall Yield Locus (or Loci)</td>
</tr>
<tr>
<td>$\Delta t$</td>
<td>Time step, s</td>
</tr>
<tr>
<td>$\mu_r$</td>
<td>Rolling coefficient of friction</td>
</tr>
<tr>
<td>$\mu_s$</td>
<td>Static coefficient of friction</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Poisson’s ratio</td>
</tr>
<tr>
<td>$\rho_s$</td>
<td>Solids density, kg m$^{-3}$</td>
</tr>
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</table>
Subscripts
p Party
p.p Particle-to-particle interaction
p.w Particle-to-boundary interaction
w Boundary or wall

8. References


