Chapter 2

Model Development and Calibration

This chapter deals with the evaluation and determination of model input parameters, and calibration of the numerical model using laboratory data. To reach the goals outlined in Chapter 1, a discrete element model that accurately simulates laboratory direct interface shear tests and that produces realistic macro and micro mechanical behavior was developed. Then the model was validated against results of laboratory tests conducted on interphase systems composed of idealized and natural particles and a variety of manufactured and natural counterfaces. The simulation data are then used to extend the laboratory data and provide a unique insight into the micromechanical behavior of the system.

The first major task of model development and calibration is the selection and evaluation of the many input parameters required in the discrete element model. These parameters include geometrical parameters, such as ratio of sample length and height to average particle diameter, number of asperities, ratio of asperity height to average particle diameter, etc., as well as physical parameters, such as normal and shear stiffness of particles and boundary walls, density and Poisson’s ratio of particles, interparticle and interface friction coefficients, etc. Each of these parameters will affect one or more certain aspects of interphase shear behavior and can cause different mechanical responses. All of them work together to influence the simulation result in a complex way. This presents a challenge to properly select each of these parameters to obtain correct and realistic mechanical behavior.

Approximately 400 laboratory direct interface shear tests have been conducted on idealized surfaces by Dove and Jarrett 2002 and on geomembranes by Dove 1996, and Dove and Harping 1997. These experimental results are used directly to calibrate the discrete element model. In addition, the model is improved by incorporation of particle rolling resistance, an important mechanism responsible for the shear banding of granular media.
2.1. Numerical Model and Sample Preparation

Model development proceeded in two stages. The first stage consisted of identifying the model variables and evaluating their impact on system behavior. The second stage was the development of a rolling resistance model that was incorporated into the final DEM model.

2.1.1. Model description

In the first stage of model development, the interphase system was composed of granular assemblage of 0.7 mm monosized spherical particles in contact with continuous regular “saw-tooth” surfaces. Geometry of the saw-tooth surface is shown in Figure 2.1(a). Independent parameters that describe the geometry of the asperities include peak to valley asperity height \( R_y \), asperity width \( S_w \) and spacing between asperities \( S_r \). Asperity slope \( \Delta_a \) can be derived from \( R_y \) and \( S_w \) using the relationship \( \tan \Delta_a = 2R_y / S_w \). In this research, \( R_y \), \( S_w \) and \( S_r \) are normalized with respect to median particle diameter \( D_{50} \) to scale the surface geometry to particles. Figure 2.1(b) shows a cross section of the final plane strain direct interface shear test model. Due to symmetry, only half of the model is shown. The model consists of a 128 mm long, 28 mm high saw tooth box filled with spherical particles with median diameter of 0.7 mm.

A 20 mm-long frictionless, non-dilative zone is placed between the asperities and side boundary walls, which minimizes the boundary influences on the interface shear behavior. The particles are modeled as “spheres” instead of “disks” or “rods” as required by the Hertz-Mindlin contact model which is subsequently discussed. In 2D simulation, it means that the assemblage is comprised of a collection of variable-diameter spheres with all their centroids lying in the same vertical plane. This is just one way of interpretation of what, in a three-dimensional sense, is being simulated in a two-dimensional model.

The sample is consolidated to equilibrium under a normal load of 100 KPa during the initial confinement stage. All walls except the top one are fixed. The top wall is mobile in the vertical direction and maintains constant normal load. All the samples are prepared to the same initial porosity of 0.1 (relative density \( D_r = 95\% \) in two dimensions) so behavior corresponds to that of a dense granular material. The relative density is calculated based on the two types of packings of monosized spheres (Figure 2.2) in two-dimensional condition which give the maximum porosity of 0.215 and minimum porosity of 0.093 respectively. Shearing occurs by
displacing all asperities comprising the bottom of the box to the left at a constant velocity of 1 mm/min. Vertical and horizontal contacting forces acting on all the asperities are summed to compute the normal and shear force generated along the interface respectively.

2.1.2. Hertz-Mindlin contact model

The Hertz-Mindlin contact model is used in this research. It is a nonlinear contact formulation based on an approximation of the theory of Mindlin and Deresiewicz 1953. This model treats the contact shear tangent stiffness as a function of normal contact force and is considered to better simulate the nonlinear contact behavior. It is only applicable to the case of spheres in contact and requires two input parameters: shear modulus $G$ and Poisson’s ratio $\nu$ of the two contacting particles. The contact normal secant stiffness $K^n$ (Itasca Inc., PFC2D manual 2002) is given by

$$K^n = \left( \frac{2\langle G \rangle \sqrt{2\tilde{R}}}{3(1-\nu)} \right) \sqrt{U^n}$$  \hspace{1cm} (2-1)

and the contact shear tangent stiffness $k'$ (denoted by a lower-case letter) is given by

$$k' = \left( \frac{2\left( \langle G \rangle^2 \left(1-\langle \nu \rangle \right) \tilde{R} \right)^{1/3}}{2-\langle \nu \rangle} \right) \left| F_i^n \right|^{1/3}$$ \hspace{1cm} (2-2)

where $U^n$ is the sphere overlap, and $\left| F_i^n \right|$ is the magnitude of the normal contact force. For particle-particle contact,

$$\tilde{R} = \frac{2R^{[A]}R^{[B]}}{R^{[A]} + R^{[B]}}$$ \hspace{1cm} (2-3)

$$\langle G \rangle = \left( G^{[A]} + G^{[B]} \right)/2$$ \hspace{1cm} (2-4)

$$\langle \nu \rangle = \left( \nu^{[A]} + \nu^{[B]} \right)/2$$ \hspace{1cm} (2-5)

and for particle-wall contact,

$$\tilde{R} = R^{[\text{particle}]}$$ \hspace{1cm} (2-6)

$$\langle G \rangle = G^{[\text{particle}]}$$ \hspace{1cm} (2-7)

$$\langle \nu \rangle = \nu^{[\text{particle}]}$$ \hspace{1cm} (2-8)
The contact normal secant stiffness \( K^n \) and contact shear tangent stiffness \( k^s \) are updated in every calculation cycle based on the latest sphere overlap \( U^n \) and normal contact force magnitude \( |F_i^n| \), respectively.

2.1.3. Model physical parameters

The physical parameters used in the simulations are described below. The density of the individual spherical particles is \( 2650 \text{ kg/m}^3 \). As reported by Dove et al. (2006), the shear modulus of the beads was found by microindentation tests to be \( 2.69 \times 10^{10} \text{ N/m} \). Poisson’s ratio of particles is 0.3. The interparticle friction coefficient is 0.5. The particle to manufactured surface boundary friction coefficient is 0.05. The friction coefficient of all other boundary walls is 0.9, except for the dead zone which is frictionless. The time step used is \( 5.0 \times 10^{-5} \text{ sec} \). Viscous (contact) damping is applied in the simulation to damp dynamic forces and achieve quasistatic solution. The critical normal and shear damping coefficients both take the value of 1.0, meaning that the dynamic force response decays to zero at the most rapid rate.

2.2. Influence of Model Variables

A study was undertaken to systematically quantify the effects of the key model variables. The variables can be classified into two broad categories: (1) Model physical variables relevant to the mechanical functioning and physical soundness of the model; and (2) Model behavioral variables relevant to the different behavior of the model due to variation in state parameters and material properties. Variables belonging to Category 1 and Category 2 are listed in Table 2.1. The purpose is to select values of these variables that will enable the model to produce global mechanical behavior as close to the laboratory test behavior as possible.

Variables in Category 1 play dominant roles in the first stage of model development and should be examined in detail. The effects of each variable are examined by performing parametric analyses using model simulations. Values of each variable are changed within a given range while keeping all others constant.

Macroscopic stress-displacement relationships obtained from each parametric study simulation were directly compared with laboratory interface shear test data for the same interphase system. The results are summarized in Table 2.2. The geometry of surface asperities
used in the simulations includes $R_i/D_{50} = 0.93$, $S_n/D_{50} = 1.86$, $\Delta_a = 45^\circ$ and $S_r/D_{50} = 0$. Unless otherwise stated, surface asperity geometry remains constant in this chapter.

<table>
<thead>
<tr>
<th>Table 2.1. Model variables divided into two categories</th>
</tr>
</thead>
<tbody>
<tr>
<td>Category 1 Variables</td>
</tr>
<tr>
<td>Length of frictionless zone</td>
</tr>
<tr>
<td>Particle shear modulus and Poisson’s ratio</td>
</tr>
<tr>
<td>Time step</td>
</tr>
<tr>
<td>Boundary friction</td>
</tr>
<tr>
<td>Damping coefficient</td>
</tr>
<tr>
<td>Particle density and strain rate</td>
</tr>
<tr>
<td>Model height</td>
</tr>
<tr>
<td>Initial fabric</td>
</tr>
</tbody>
</table>

Among the eight variables in the first category, four were found to have the greatest influence on the system behavior in terms of model physical soundness. The length of frictionless zone is essential for obtaining the correct overall stress-displacement behavior with respect to the lab test results and eliminating the undesired boundary effects on the system behavior. Boundary friction controls the initial stiffness of the interface behavior. Model height allows the full development of shear band inside the sample. Initial fabric has large influence on the interface behavior. Because of the importance of these variables, their effects are described below in detail.

A limited investigation of the variables in Category 2 was also conducted at this stage. This offered a preliminary, qualitative description of their effects on global mechanical behavior, as summarized in Table 2.3. More details will be given when parametric studies are discussed later in Chapter 5.

It should be mentioned that all of the simulations are performed with particle rolling resistance incorporated into the micromechanical model. Rolling resistance will be discussed later in this chapter.
Table 2.2. Influence of Model Physical Variables—Summary

<table>
<thead>
<tr>
<th>Variables</th>
<th>Length of frictionless zone (mm)</th>
<th>Shear modulus (GPa)</th>
<th>Poisson’s ratio</th>
<th>Particle density (kg/m$^3$)</th>
<th>Strain rate (mm/min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Values tested</td>
<td>Zero frictionless zone (Model type 1)</td>
<td>26.9</td>
<td>0.3</td>
<td>2400</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>20 mm frictionless zone at both ends of the box (Model type 2)</td>
<td>29$^*$</td>
<td>0.15$^*$</td>
<td>2650</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>43 mm frictionless zone at both ends of the box (Model type 3)</td>
<td>2650000$^*$</td>
<td></td>
<td></td>
<td>10</td>
</tr>
<tr>
<td></td>
<td>Higher for Model type 1; close to lab data for Model type 2 and 3</td>
<td>Little effect</td>
<td>Little effect</td>
<td>Increases when large particle density</td>
<td>Increases slightly with large strain rate</td>
</tr>
<tr>
<td>Effects on system behavior</td>
<td>Higher for Model type 1; close to lab data for Model type 2 and 3</td>
<td>Agree better with lab data for the 29GPa case</td>
<td>Little effect</td>
<td>Little effect</td>
<td>Little effect</td>
</tr>
<tr>
<td></td>
<td>Slightly stiffer in Model type 1 and 3 than in Model type 2, but all are less stiff than lab data.</td>
<td>Little effect</td>
<td>Decreases with decreasing Poisson’s ratio</td>
<td>Little effect</td>
<td>Little effect</td>
</tr>
<tr>
<td></td>
<td>More stress fluctuations in Model type 1 and 3; excellent agreement with lab data in Model type 2</td>
<td>Little effect</td>
<td>Little effect</td>
<td>Large improvement of computation efficiency achieved by increasing particle density and strain rate simultaneously provided that particle acceleration is close to zero and quasi-static solution is valid. Final values used in this research: particle density 2650000 kg/m$^3$ and strain rate 30mm/min</td>
<td></td>
</tr>
</tbody>
</table>

*Note: Values marked with an asterisk (*) indicate specific conditions or calculations relevant to the model's behavior.
Table 2.2. Continued

<table>
<thead>
<tr>
<th>Variables</th>
<th>Time step (s)</th>
<th>Boundary friction</th>
<th>Damping coefficient</th>
<th>Model height (mm)</th>
<th>Initial fabric</th>
</tr>
</thead>
<tbody>
<tr>
<td>Values tested</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$5 \times 10^{-4}$</td>
<td>0.05</td>
<td>0.15</td>
<td>7</td>
<td>Interparticle friction coefficient used during consolidation: 0.05 and 0.5, giving isotropic and anisotropic fabric respectively</td>
</tr>
<tr>
<td></td>
<td>$5 \times 10^{-5}$</td>
<td>0.9</td>
<td>1.0</td>
<td>14</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$5 \times 10^{-6}$</td>
<td></td>
<td>1.5</td>
<td>21</td>
<td></td>
</tr>
<tr>
<td>Effects on system behavior</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Peak stress ratio</td>
<td>Little effect</td>
<td>Little effect</td>
<td>Little effect</td>
<td>Little effect</td>
<td>Little effect; More consistent behavior observed with initial isotropic fabric; Finite initial built-in stress more likely associated with initial anisotropic fabric</td>
</tr>
<tr>
<td>Steady state stress ratio</td>
<td>Little effect</td>
<td>Little effect</td>
<td>Best agreement with lab data found in the 1.0 case</td>
<td>Little effect</td>
<td></td>
</tr>
<tr>
<td>Initial stiffness</td>
<td>Little effect</td>
<td></td>
<td>Little effect</td>
<td>Decreases with increasing model height</td>
<td>Lower for anisotropic fabric</td>
</tr>
<tr>
<td>Stress fluctuation</td>
<td>Equilibrium not achieved in the $5 \times 10^{-4}$ case</td>
<td>Little effect</td>
<td>Improved stability in the 1.0 case</td>
<td>Little effect</td>
<td>More stress fluctuations for anisotropic fabric</td>
</tr>
</tbody>
</table>

Note: Values marked with * were suggested by Ng 2004 through personal communication.
Table 2.3. Influence of Model Behavioral Variables-Summary

<table>
<thead>
<tr>
<th>Variables</th>
<th>Confining pressure (KPa)</th>
<th>Initial relative density (%)</th>
<th>Particle size distribution ($D_{max}/D_{min}$)</th>
<th>Interparticle friction coefficient</th>
<th>Particle to surface friction coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>Values tested</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>15 50 100 200 300</td>
<td></td>
<td>95 80</td>
<td>1.0 1.1 1.7 3.0</td>
<td>0.2 0.5 0.8 0.2</td>
</tr>
<tr>
<td>Effects on system behavior</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Peak stress ratio</td>
<td>Decreases with increasing confining pressure</td>
<td>Increases with increasing initial relative density</td>
<td>Higher for well-graded material</td>
<td>Increases with increasing interparticle friction coefficient</td>
<td>Increases with increasing particle to surface friction coefficient</td>
</tr>
<tr>
<td>Steady state stress ratio</td>
<td>Little effect</td>
<td>Little effect</td>
<td>Little effect</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Initial stiffness</td>
<td>Decreases with increasing confining pressure</td>
<td>Little effect</td>
<td>Little effect</td>
<td>Little effect</td>
<td>Little effect</td>
</tr>
<tr>
<td>Stress fluctuation</td>
<td>Little effect</td>
<td>Little effect</td>
<td>Less fluctuations with well-graded material</td>
<td>Little effect</td>
<td>Little effect</td>
</tr>
</tbody>
</table>
2.2.1. Length of frictionless, non-dilative zone

Three model types with different length of a frictionless, non-dilative zone have been tested. Model type 1 has continuous asperities distributed across the full length of the box and no frictionless zone. Model type 2 [Figure 2.1(b)] has 20 mm long frictionless zones placed at each end of the box. The reminder of the lower boundary is composed of continuous asperities. Model type 3 differs from Model type 2 in that its length of the frictionless zone at either end is 43 mm, approximately 1/3 of the box length. The global stress-displacement relationships obtained from three simulations using the three model types are shown in Figure 2.3.

It can be seen that the overall shape of the stress-displacement curve for Model Type 2 agrees best with the lab test results. For Model type 1, the peak stress ratio is higher than the lab test data and occurs at relatively larger displacement. This is due to the stress concentration at the left lower corner of the box when surface asperities squeeze the particles against the lateral boundary. The lack of frictionless zone causes this artificial boundary effect and leads to unrealistic behavior. This effect is found to be magnified in shorter samples.

In Model type 3, a severe stress fluctuation is observed after peak state, due to insufficient number of asperities. Considering the geometric and boundary effects on the system behavior, Model Type 2 is most suitable for DEM simulation of a direct interface shear test.

In principle, for realistic simulation of interphase shear behavior, the model should have surface asperities covering as much of its full length as possible, while trying to minimize the undesirable boundary effects created in the numerical simulation. In addition, the constraint imposed by the lateral and top boundary increases when the model size decreases. More details regarding boundary influence will be given in the discussion of next two variables.

2.2.2. Boundary friction

Boundary friction has significant influence on global mechanical behavior. Two simulations with roughened and smooth boundaries were conducted by applying particle to wall friction coefficient of 0.9 and 0.05 to the top and lateral walls. The results are shown in Figure 2.4. The stiffness of interface shear before peak state is found to be lower in the smooth boundary case than that in the roughened boundary case. This is because the smooth boundary allows the whole assemblage to travel in the shear direction with nearly the same velocity, while the roughened boundary prevents this motion of the entire assemblage, leaving only particles
near the surface to travel with higher velocity, as evident from the distribution of particle velocity vectors at 1 mm shear displacement shown in Figure 2.5.

Besides initial interface stiffness, different dilation behavior is another consequence of boundary friction. Figure 2.6 compares the variations of vertical displacement of top wall with shear displacement in the two boundary friction cases. Greater dilation is observed in the roughened boundary case up to post-peak state (around 2 mm displacement). After that, greater dilation occurs in the smooth boundary case until steady state. This indicates that the roughened boundary better prompts the dilation behavior before post-peak state, and therefore should be adopted in our model for realistic simulation of both macro and micro mechanical interphase behavior.

The above effects are found to be more pronounced in smaller sized models, as similar to the case of variable 1. This is because smaller number of particles exists in the smaller sample and they are more likely to “feel” the constraint imposed by the boundary.

2.2.3. Model height

Model height was found to be critically important to the micromechanical behavior of the interphase system, but have less influence on the overall stress-displacement behavior. Figure 2.7 shows the results of four simulations with model height varying from 7 mm to 35 mm. No distinct change was observed on the peak and steady state stress behavior, but the initial interface stiffness before peak state was found to decrease with increasing model height. This is a result due to the attenuated influence of top boundary friction on the interface behavior in thicker models.

The most significant effects of model height exist on the shear banding behavior of the interphase soils. The thickness of the shear band was found to scale with the model height, with the maximum thickness occurring at a model height of 40 to 50 $D_{50}$. The evolution of shear band will be artificially restrained in a shorter model. However, the overall deformation pattern remains the same regardless of model height. More details will be given in Chapter 3.

2.2.4. Initial fabric

Initial fabric refers to particle arrangement and distribution of particle contact normals in varying orientations inside the granular media before shearing starts. Samples can be formed
with isotropic or anisotropic initial fabrics at the end of consolidation. Fabric can be said to be isotropic when the distribution of contact normals is approximately the same in all orientations. Anisotropic fabric results when the average contact normal orientations are not uniformly distributed. The parameter controlling material fabric after consolidation is the interparticle friction coefficient used during the consolidation stage. It was found that a more symmetric fabric is achieved if a small interparticle friction coefficient during consolidation was adopted. The resulting initial porosity (or void ratio) is lower. Global behavior consistent with the laboratory tests was observed when samples had a symmetric initial fabric. When a higher interparticle friction coefficient is used during consolidation, a less symmetric fabric typically results. This non-symmetry state will usually lead to a finite initial shear stress, and require more energy to rearrange the particles to reach a steady state fabric. As a result, a greater number of stress fluctuations are observed for a sample with initial anisotropic fabric before steady state is reached. Figure 2.8 shows a relatively initial symmetric and a relatively initial asymmetric fabric resulting from interparticle friction coefficient of 0.0 and 0.5 during consolidation, respectively. Figure 2.9 shows their stress-displacement curves.

Based on the above observations, it is recommended that a small interparticle friction coefficient be used during consolidation to achieve relatively symmetric fabric for a dense or medium dense sample. In some cases, it is necessary to use high interparticle friction coefficient to prepare a sample with low initial density under a specified confining pressure. Under these circumstances, the effects of asymmetric fabric are unavoidable.

2.3. Direct Shear Test Simulation

Interphase strength ultimately depends on the strength of the granular component. Therefore interphase strength is often expressed in terms of an efficiency factor, $E$ (Koerner 1990), which normalizes interface strength with respect to the granular material strength. For coarse-grain particulate materials, $E$ is defined as $E = \tan \delta / \tan \phi$, where $\tan \delta$ is the effective stress interphase friction coefficient and $\tan \phi$ is the effective stress friction coefficient of the particulate material alone. Efficiency can be defined in terms of peak state or steady-state strengths. Therefore, to compute $E$, it is necessary to obtain the strength of the granular assemblage using a simulated direct shear test.
The direct shear test model shown in Figure 2.10 is 88 mm long, 56 mm high, and composed of upper and lower halves. Constant normal stress is exerted on the top of the upper half which is stationary during the test; while the lower half moves toward right to shear the sample. Triangular-patterned saw teeth are used at the top and bottom of the box to prevent slip between the sample and the boundaries. Both well graded and uniformly graded materials were used in the simulations. Figure 2.10 shows the typical internal deformation of a dense well graded sample after 10 mm shear displacement. Chapter 4 provides detailed information regarding shear banding behavior in the direct shear test. The direct shear test model is validated by comparing the simulation results of a uniformly graded material to laboratory data. Figure 2.11 shows the stress-displacement curves. The peak and steady state stress ratios from the simulation agrees well with the data from a similar test in the laboratory.

2.4. Incorporation of Particle Rolling Resistance

The PFC2D code used in the research allows for free rotation of soil particles during deformation. While free rotation may correctly model some particle flow regimes, it is not realistic for quasi-static deformation of soil. Research over the past 20 years has demonstrated the significance of particle rolling resistance in the micromechanical simulation of strain localization in shear bands developed in granular materials. Therefore it is a major component of our model development to incorporate particle rolling resistance in PFC2D.

2.4.1. Previous related work

In the past few decades, a number of research works have been reported on the role of particle rolling in the strain localization of granular soils. Oda et al. 1982 pointed out that particle rolling, as compared to sliding, is an important microscopic mechanism when interparticle friction is large. In their experimental observations, Oda and Kazama 1998 noted large voids and high gradient of particle rotation were generated inside the shear band, which can not be reproduced using any conventional numerical method. Therefore, in the same paper, they suggested that rolling, instead of sliding, is the dominant microdeformation mechanism controlling the dilatancy taking place inside a shear band. Iwashita and Oda 1998 proposed a modified discrete element method taking into account the rolling resistance and concluded that the new method better reproduces the microstructure developed in the shear band observed in the
laboratory tests by Oda and Kazama 1998. Bardet 1994 demonstrated in his numerical simulation of a biaxial test that particle rotations have significant effects on shear strength of idealized granular material, although it has little effects on the elastic properties (Young’s modulus and Poisson’s ratio). He pointed out that the overall peak and residual friction angles are smaller than interparticle friction angle due to high concentration of rotations in shear bands. This is because, from the micromechanical point of view, the rolling contacts are much less capable of supporting oblique contact forces, creates less particle interlocking and dissipates less energy than sliding contacts. In presence of rolling resistance, overall peak and residual friction angles may equal or exceed the interparticle friction angle.

However, there is presently little information with regard to particle rolling resistance on the interface shear behavior of granular material. Therefore, a study has been conducted to examine the influence of rolling resistance on interface systems composed of ideal spheres in contact with regular saw tooth surfaces. Specifically, the overall shear strength ratio and stress-displacement behavior is investigated and compared with the free rolling case. Laboratory data on interface shear tests are used to demonstrate the importance of incorporating this mechanism. A paper by Wang et al. 2004 has reported these results.

2.4.2. Rolling resistance model at contacts

The rolling resistance model developed by Iwashita and Oda (1998) as presented below is used in this research. It is implemented in the Discrete Element Method (DEM) proposed by Cundall 1971.

Consider a particle with a radius $r$ surrounded with $n$ contacts. At the $i$th contact, the contact force $F_i$ can be decomposed into a normal component $N_i$ and a shear component $T_i$. Two types of kinematical behavior can occur for a contact: sliding and rolling. Sliding occurs when the shear component $T_i$ exceeds the shear strength $T_{i_{\text{max}}}$ of the contact, which is defined as:

$$T_{i_{\text{max}}} = \mu \cdot |N_i|,$$  \hspace{1cm} (2-9)

where $\mu$ is the friction coefficient of the contact.

In conventional DEM, rolling of particle occurs without any resistance. The conservation law of angular momentum can be expressed by the following relation:

$$\sum_{i=1}^{n} T_i r = I \frac{d\omega}{dt},$$  \hspace{1cm} (2-10)
where \( I \) and \( \omega \) are the moment of inertia and angular velocity of the particle respectively. However, in reality particles contact neighboring particles at contact surfaces with finite area and thus a moment of rolling resistance exists when a particle rolls over another. Denoting the moment of rolling resistance by \( M_i \), then equation (2-10) becomes:

\[
\sum_{i=1}^{n} (T_i r + M_i) = I \frac{d\omega}{dt}.
\]  

(2-11)

This model consists of an elastic spring, a dash pot, a no-tension joint and a slider which provide two sources of rolling resistance:

\[
M_i = -k_r \theta_r - C_r \frac{d\theta_r}{dt},
\]

(2-12)

where, \( k_r \) is the rolling stiffness, \( C_r \) is the viscosity coefficient, and \( \theta_r \) is the relative rotation between two particles. \( C_r \) is set equal to zero in the present model as the second term of equation (2-12) only serves to stabilize the numerical computation and has little effect on the results. It is assumed that if \( M_i \) exceeds a threshold value \( \eta N_i \), a particle just starts to roll without mobilizing any further rolling resistance:

\[
M_i \geq \eta N_i.
\]

(2-13)

where \( \eta \) is the coefficient of rolling resistance first defined by Sakaguchi 1993. The value \( \eta = 10^{-5} \) is used in this study. Bardet and Huang 1993 derived the analytical expression of \( k_r \) as:

\[
k_r = -2rN_i J_n,
\]

(2-14)

where \( J_n \) varies from 0.25 to 0.5. Since perfectly rigid spherical particles are used in the current simulation, \( J_n \) takes the value of 0.5.

### 2.4.3. Effects of rolling resistance on stress-displacement behavior

Figure 2.12 compares the stress-displacement relationships from three simulations with rolling resistance and free rolling respectively. The saw tooth surfaces used in the three simulations have asperity slopes of 20, 30 and 45 degrees. The general shapes of the stress ratio-displacement curves from numerical simulations resemble those from the laboratory tests. However, particle rolling resistance improves the overall shapes of these curves and makes them agree better with the laboratory results, especially for the 20 and 45 degree cases. It should be mentioned that the results shown here are different from those presented by Wang et al. 2004.
Some changes have been made on the model physical variables after the paper was published, including model width increase from 64 mm to 128 mm, model height increase from 7 mm to 28 mm and boundary friction increase from 0.05 to 0.9. So a much smaller sample was used by Wang et al. 2004, which certainly imposes much greater boundary effects on the results. But the major conclusions regarding the effects of rolling resistance remain the same.

2.4.4. Effects of rolling resistance on shear strength

As shown in Figure 2.12, rolling resistance does not change the initial slopes of the curves, indicating it has little effect on the Young’s modulus of the granular material, but it definitely shows a significant effect on the peak stress behavior. Compared to the free rolling case, the peak stress ratios increase about 5, 6, 14 and 17 percent for 10, 20, 30 and 45 degree asperity slopes, respectively. These observations are in agreement with Bardet 1994. The inclusion of rolling resistance makes it harder for particles to roll over the asperities after shearing starts. Peak resistance is obtained when particles begin to roll over the asperities. The average normal contact force inside the shear band is larger in rolling resistance case than in free rolling case. Rolling resistance shows a much greater influence on the peak strength in the high asperity slope cases than in the low asperity slope cases. For low asperity slopes (≤ 20 degrees), a greater percentage of particles are sliding over the asperities thus the influence of rolling resistance is low. For high asperity slopes (> 20 degrees), particles are less able to slide over the asperities and rolling becomes a prevailing deformation mode when peak resistance is reached. Some particles are trapped within the valleys of the asperities and travel with the lower surface. In this instance, the shear strength of granular material will most likely be mobilized.

At the steady state, the granular material is continuously deforming at constant shear stress ratio and constant volume. As compared to the peak stress ratio, only slight increase can be observed in the steady state stress ratios with rolling resistance for all the simulations. The smaller effect of rolling resistance on steady state stress ratios may be because the number of sliding contacts increases as compared to that of rolling contacts.

2.4.5. Effects of rolling resistance coefficient $\eta$

The coefficient of rolling resistance, $\eta$, has important effects on the mechanical response of the interface system. Several numerical tests were performed using different values of $\eta$ for
different asperity slopes. It is discovered that high values of $\eta$ produce high peak stress ratio and a reduction in $\eta$ value lowers both the peak and steady state stress ratios. There is a narrow range within which coefficient of rolling resistance influences the peak and steady state stress ratio in a reasonable way and makes the stress response of the whole system more close to the real case. Unfortunately, to date, there is no method to compute the value of $\eta$ for a specific problem.

The following procedure to determine $\eta$ was used in this study: 1) In the free rolling case, record the average normal contact force $N_{ave}$ and shear contact force $T_{ave}$ of the sample at the peak stress ratio; 2) Treat the moment induced by the average shear contact force $T_{ave}$ on a single particle as $M_{max}$, thus $M_{max} = T_{ave} \cdot r$; 3) Estimate $\eta$ from the following equation:

$$\eta = \frac{M_{max}}{N_{ave}} = \frac{T_{ave} \cdot r}{N_{ave}}$$

and 4) Adjust $\eta$ as necessary.

2.4.6. Micromechanical behavior

Within the granular media, volume change is mainly caused by the increase in void space between the particles. Figure 2.13 shows the void distribution inside the sample for the rolling resistance and free rolling cases at 5 mm shear displacement. In the rolling resistance case, voids are largely concentrated in the shear zone above the surface [Figure 2.13(a)]. In contrast, a nearly uniform distribution of voids without any particular alignment is observed in the free rolling case [Figure 2.13(b)]. This agrees with Oda and Kazama’s observation 1998 in the biaxial simulation of shear band in granular soil. Besides the void distribution, different amounts of dilation in the two cases are also observed. Figure 2.14 shows that for all the asperity slope cases, the dilation of the sample indicated by the vertical displacement of the top wall is much greater in the rolling resistance case than that in the free rolling case. It can be easily explained by particle rolling resistance which prevents particles from rolling over each other easily and causes arching action at contacts. This mechanism makes major contribution to the dilatancy characteristics of the granular material at peak and steady state phase. At the steady state phase, the volume of the sample remains nearly a constant. This indicates that rolling resistance is the dominant mechanism responsible for the dilation of the granular material.

Another remarkable effect of rolling resistance is its role on the evolution of shear band. Before the peak stress state, the sample is deforming uniformly. Columns of particles tend to
rotate clockwise slightly as a whole. After peak state, deformations localize into a few shear bands. But the details of strain localization are different, depending on the models adopted. Figure 2.15 shows the shear strain distributions inside the sample for the rolling resistance case and free rolling case, recorded at 2 mm and 5 mm shear displacement. The details of the shear strain calculation will be addressed in Chapter 3. It is surprising to find that a distinct shear band is formed in the rolling resistance case while almost no clear shear band exists in the free rolling case. However, this observation totally agrees with those by Oda and Kazama 1998, who pointed out that the high mobility of particles, not only by rolling but also by sliding, makes them possible to move along many shear zones. As a result, strains do not concentrate in any specific zone in the free rolling case [Figures 2.15(b) and (d)]. In contrast, strain localization is concentrated in the narrow region above the surface in the rolling resistance case, as shown in Figures 2.15(a) and (c). This is the same region where most of voids are distributed [Figures 2.13(a)], indicating dilation is concentrated inside the shear band.

2.5. **Summary**

This chapter deals with the development and calibration of the DEM model of direct interface shear test using PFC2D. Parametric studies were conducted to find out the effects of model physical variables and behavioral variables on system behavior and to determine the most appropriate values for the realistic simulation of the macroscopic as well as microscopic interphase behavior.

Four model physical variables, namely length of frictionless zone, boundary friction, model height and initial fabric are identified which show significant influences on the system behavior. The first three variables are found to affect the model behavior through imposing the boundary constraint in different ways. Therefore, it is an important conclusion of the author now that the boundary effect, besides elastic properties of granular particles and surfaces, plays an essential role in the correct and realistic simulation of interphase behavior.

Particle rolling resistance has great importance on both the macroscopic and microscopic interphase shear behavior. It raises the peak strength ratio of the interphase system. The effect is also more pronounced for high asperity slopes than for low asperity slopes. The greater dilation from the large voids generated inside the shear band demonstrates that particle rolling resistance is a major factor governing the dilatancy characteristics of the granular interphase system. More
importantly, rolling resistance plays an essential role in the evolution of the shear band, which is practically invisible in the free rolling case. In the region of strain localization, concentrated distribution of voids is observed with rolling resistance.

**Notation**

*The following symbols are used in this chapter:*

- $C_r$ = viscosity coefficient of contacts
- $D_{50}$ = median particle diameter (mm)
- $D_r$ = relative density
- $E$ = Young’s modulus of particles
- $F_i$ = contact force at the $i^{th}$ contact
- $|F_i^n|$ = magnitude of normal contact force
- $G$ = particle shear modulus
- $I$ = moment of inertia of particles
- $J_n$ = rigidity parameter for determination of rolling stiffness
- $K^n$ = contact normal secant stiffness
- $k_r$ = rolling stiffness of particles
- $k^s$ = contact shear tangent stiffness
- $M_i$ = moment of rolling resistance
- $N_i$ = normal component of contact force $F_i$
- $R$, $r$ = particle radius (mm)
- $R_i$ = asperity height ($\mu$m)
- $R_{ave}$ = average value of maximum asperity height over a series of assessment lengths, $L$ (mm)
- $R_{max}$ = maximum accumulated asperity height (mm)
- $S_r$ = spacing between asperities (mm)
- $S_w$ = asperity width (mm)
- $T_i$ = shear component of contact force $F_i$
- $U^n$ = sphere overlap
- $\delta$ = effective stress interface friction angle (degrees)
- $\Delta_s$ = asperity slope
\( \phi \) = effective stress friction angle of granular media (degrees)
\( \eta \) = coefficient of rolling resistance
\( \mu \) = friction coefficient between particles
\( \nu \) = Poisson's ratio of particles
\( \theta_r \) = relative rotation between two particles
\( \omega \) = angular velocity of particles

References


Figure 2.1. Numerical model composed of densely packed spheres in contact with a rough saw-tooth surface: (a) geometry of saw-tooth surface; (b) DEM model of plane strain direct interface shear test.
Figure 2.2. Two-dimensional packings of monosized spheres giving the maximum and minimum porosity: (a) simple square (corresponding to simple cubic in three dimensional case) with maximum porosity of 0.215; (b) hexagonal with minimum porosity of 0.093.
Figure 2.3. Stress-displacement relationships for different model types: (a) Model type 1 without frictionless zone; (b) Model type 2 with 20 mm long frictionless zones at each end of the box; (c) Model type 3 with 43 mm long frictionless zones at each end of the box.
Figure 2.4. Stress-displacement relationships in different boundary friction cases: (a) particle to boundary friction coefficient 0.9; (b) particle to boundary friction coefficient 0.05.
Figure 2.5. Distributions of particle velocity vectors at 1 mm shear displacement in different boundary friction cases: (a) particle to boundary friction coefficient 0.9; (b) particle to boundary friction coefficient 0.05.
Figure 2.6. Variations of vertical displacement of top wall with shear displacement in different boundary friction cases.
Figure 2.7. Stress-displacement relationships for different model heights: (a) 7 mm high model; (b) 14 mm high model; (c) 28 mm high model; (d) 35 mm high model.
Figure 2.8. Initial fabrics (contact normal distributions) resulting from different interparticle frictions during consolidation: (a) interparticle friction coefficient 0.0 during consolidation; (b) interparticle friction coefficient 0.5 during consolidation.
Figure 2.9. Stress-displacement relationships for different initial fabrics: (a) interparticle friction coefficient 0.05 during consolidation resulting in isotropic initial fabric; (b) interparticle friction coefficient 0.5 during consolidation resulting in anisotropic initial fabric.
Figure 2.10. Direct shear test model with typical internal deformation at 10 mm shear displacement.
Figure 2.11. Comparison of stress-displacement curves from a direct shear test simulation and a similar laboratory test.
Figure 2.12. Comparisons of stress-displacement relationships for rolling resistance and free rolling cases: (a) 20 degree asperity slope; (b) 30 degree asperity slope; (c) 45 degree asperity slope.
Figure 2.13. Distributions of voids inside the sample for rolling resistance and free rolling cases:
(a) rolling resistance; (b) free rolling.
Figure 2.14. Variations of vertical displacement of top wall with shear displacement for rolling resistance and free rolling cases: (a) 20 degree asperity slope; (b) 30 degree asperity slope; (c) 45 degree asperity slope.
Figure 2.15. Shear strain distributions inside the sample for rolling resistance and free rolling cases: (a) and (c) rolling resistance, recorded at 2 mm and 5 mm shear displacement respectively; (b) and (d) free rolling, recorded at 2 mm and 5 mm shear displacement respectively.