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PREDICTION OF DISCRETE ELEMENT PARAMETERS FOR MODELING THE STRENGTH OF SANDY SOILS IN WHEEL/SOIL TRACTION APPLICATIONS

Timothy Reeves
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PREDICTION OF DISCRETE ELEMENT PARAMETERS
FOR MODELING THE STRENGTH OF SANDY SOILS
IN WHEEL/SOIL TRACTION APPLICATIONS

A Dissertation
Presented to
the Graduate School of
Clemson University

In Partial Fulfillment
of the Requirements for the Degree
Doctor of Philosophy
Mechanical Engineering

by
Timothy C. Reeves
May 2013

Accepted by:
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ABSTRACT

The problem of wheel performance on deformable soil has been studied for many years, but prior to the rise of computational mechanics, such investigations have been limited to development of analytical and empirical models, as well as experimental research. Such models have merit but are necessarily highly idealized and are limited in their applications. Today, many computational models have been implemented for a wide variety of wheel/soil applications.

For the specific case of sandy (i.e. non-cohesive) soils, in terms of the soil’s physics the Discrete Element Method (DEM) provides arguably the most realistic model. In DEM, each element represents a single grain of soil (ideally), or may represent a group of soil particles moving together if necessary. A survey of the literature quickly reveals that DEM is computationally intensive and that a great deal of computational effort is normally spent calibrating the DEM model parameters to the desired characteristics of the soil of interest. The goal of this research was to develop and validate an approach to calibration that would require fewer resources, leaving more resources available for solving the problems of interest. This goal was realized through the collection of data over a range of values for each of five simulation parameters using two-dimensional simulations of the Direct Shear Test. By statistical processes the data was used to develop a set of equations that estimate the properties of interest for the simulated soil (small- and large-strain friction angles), based on the simulation parameters. The equations were used to calibrate a two-dimensional rigid wheel/soil simulation of the Wheel Endurance and Sand Traction Merry-Go-Round System (WEST-MGRS). The
calibrated model was found to accurately predict the relative performance between a variety of configurations of grousers on actual wheels operating in sand using WEST-MGRS. Therefore, this research shows that the model can be used as a tool to compare the tractive performance of potential designs.

A question that must be answered regarding experiments and simulations of the wheel/soil problem is the question of soil dimensions. Whether simulated or experimental, the system must use a soil container large enough to approximate a semi-infinite soil domain. This research expanded on previous work that had proposed a method for sizing soil dimensions in a dynamic 3-D finite element model. With minor modifications, the method was found to be effective for a wide range of wheel loads and geometries, as well as soil types.
DEDICATION

This project is dedicated to certain dear people in my life.

John and Glenda: Without you I likely would not have started.

All my parents: Without you I likely would not have kept going.

Anna: Without you I likely would not have finished.

Jesus Christ: “…without [You], [I] can do nothing.” (John 15:5, NKJV)
ACKNOWLEDGMENTS

The number of people who have contributed to my success is large enough that I do not have space to name them all. To those not named: your support has not been taken for granted. Thank you.

Dr. Sherrill Biggers has not only provided oversight to my research project, but has more importantly done so in such a way that has forced me to grow as a person. He has not held my hand (as perhaps I would have been more comfortable with) but rather has given me a great deal of freedom to take ownership and responsibility of the project. As a result I believe that I am far better prepared to leave my life as a student than I would have been otherwise. Similarly, each member of my committee has expressed confidence in the work that I have done as well as a commitment to making me a success. I am deeply indebted. Furthermore, special thanks to Dr. Joshua Summers for going above and beyond his basic committee-member duties to offer informal mentorship that tended to infringe on his personal time.

Peer support has been a big encouragement even though nobody else was doing anything with DEM. Dr. Marisa Orr has repeatedly encouraged me, given me creative suggestions, and offered examples of successful work for guidance. Several members of the CEDAR lab have offered moral support and assistance with computer issues. I enjoyed having the help of EUREKA students Elizabeth and Isaac.

Finally the work would not have been possible without research funds. I am grateful to the Automotive Research Center, NASA, and the South Carolina Space Grant for entrusting me to model sand for you. Thank you for the opportunity.
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1. MOTIVATION

Two-dimensional Discrete Element Method (DEM) modeling was introduced to the Mechanical Engineering Department as part of an effort to establish a suite of experimental and computational tools to predict the interaction of deformable wheels such as the Michelin Tweel® with dry sandy soils such as those found in the desert or on the moon. This goal was motivated by grants from the Automotive Research Center (ARC) and the National Aeronautics and Space Administration (NASA), both of which are interested in wheeled locomotion in sandy soils (re: NASA, see Figure 1.1); then later the South Carolina Space Grant Consortium contributed funding because of the project’s relevance to lunar exploration. It was found that much work had been published on the interaction of wheels and soft soil, but most had been applicable to clay-dominated (i.e. cohesive) soils. This was because almost all modeling (analytical and finite element) had been done under the assumption of soil as a continuum, thereby excluding much of the detail of the sandy soil’s behavior on the length scale of individual particles. Since DEM is not a continuum-based model, but rather treats systems as a collection of independent, discrete particles that interact with each other through contact, it is able to capture much of the detail that escapes the analytical and finite-element soil models. This advantage was demonstrated by some preliminary DEM simulations, and the decision was made to purchase a 2-D DEM software package (PFC\textsuperscript{2D}) in order to further expand the research group’s capabilities.
Figure 1.1: Wheel of NASA’s Mars Exploration Rover “Spirit” partially buried in Martian sand on Dec 12, 2009 (http://www.jpl.nasa.gov/freespirit/free-spirit-archive.cfm). Spirit remained entrapped until Mar. 22, 2010, when the low solar power of the Martian winter caused the rover to enter a hibernation mode. The rover has not yet resumed communication with Earth and is assumed to be still trapped.

Once extensive DEM work began it became clear that the computational requirements of the method made it impractical to attempt a true-particle-size DEM simulation of a sand bed large enough to include the volume of soil that would be affected by a rolling wheel. To address this problem, the idea of a coupled Discrete/Finite Element Method (DEM/FEM) simulation was discussed as a possible solution. The DEM would model the soil immediately in contact with the wheel, and the FEM would model the rest of the soil (which would undergo much less extreme deformation) as well as the deformable wheel (essentially a continuum on the length scale of interest). To develop such a model with accuracy (as with any DEM model), calibration simulations needed to be performed to determine appropriate input parameters for the DEM particles. A significant simulation effort was invested toward calibration, covering a significantly broader range of input parameters than needed for this project. This extra work was performed to produce results that would be useful in guiding the
calibration of future DEM projects as well as this one. This required a great deal of computational time and calendar time. As the calibration process neared completion, it was recognized that the task of developing a coupled DEM/FEM simulation in addition to the calibration effort was beyond the scope of a single Ph.D. dissertation. Therefore that task was excluded from the scope of this project.

During the course of the team’s research, the question of 2-D versus 3-D wheel/soil simulations continued to be raised. Evidence was found in the literature [1] and in the group’s own FEM simulations that the 3-D effect may be significant in this problem and that 2-D simulations may not be accurate. However, these conclusions are based on continuum-based simulations. Therefore a comparison of the wheel/soil interaction problem using DEM in 2-D and in 3-D is of great interest. This question remains as one of the objectives of related future work as described in Chapter 7.

During discussion of the 2-D vs. 3-D question, the team recognized that a great deal of useful knowledge had yet to be extracted from the vast array of data that had already been collected from the calibration process, and that the extraction of that knowledge would be a non-trivial process. Hence this became a primary focus of the research described in this dissertation.

In addition to the DEM work, studies were being done in parallel on a different aspect of the problem. Any physical or computational model of a wheel/soil problem must include an appropriately sized volume of soil in order to approximate the behavior of a semi-infinite domain. A thorough evaluation of the general applicability of the soil domain sizing method previously proposed by Orr, et. al. [2] was conducted using Finite
Element Analysis. This information will contribute to the ultimate goal (beyond the scope of this dissertation) of developing a coupled FEM/DEM model of the wheel/soil problem.

The goals of this research project are expressed in terms of several research questions, found in Table 1.1.

Table 1.1: Research Questions

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<th>RQ1</th>
<th>How do the parameters of friction coefficient, dyad eccentricity, normal contact stiffness, shear contact stiffness, porosity, rate of shear, and upscale factor influence the shear strength of a simulated sand in DEM?</th>
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<td>RQ2</td>
<td>Can a large body of data collected from simulations using a variety of DEM parameters be used to fit a statistical model that will enable the direct selection of appropriate parameters to achieve specific desired system behavior?</td>
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<td>RQ3</td>
<td>Can a 2-D wheel/soil model in DEM be used to compare the performance of different grouser configurations and predict which one(s) will develop superior traction in sand?</td>
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<td>RQ4</td>
<td>Does the soil sizing method proposed by Orr work for a wide variety of systems?</td>
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2. LITERATURE REVIEW

The work of Bekker has served as a starting point for almost all wheel/terrain modeling over the past fifty years (i.e. most authors on this topic reference his work). Bekker developed analytical and empirical equations to predict typical quantities of interest for traction, including drawbar pull, rolling resistance, and sinkage [3]. He considered the behavior of rigid and deformable wheels on soft soil as well as the behavior of tracked vehicles. However, he gave minimal treatment to the influence of grousers on wheel performance, a topic important to the current study; further, regarding Bekker’s treatment of grousers, it is not clear whether the conclusions are applicable for a particular type of soil or for all types. This topic pertains directly to Chapter 5 of this dissertation, which deals primarily with the performance of rigid, grousered wheels on sandy soil.

More recently computational methods have been recognized as a promising approach to the complexity of the wheel/soil problem. Two-dimensional finite element wheel/soil models were developed by Ma et al (non-pneumatic deformable tire with deformable but comparatively stiff soil) [4], Schmid (deformable pneumatic tire and similarly stiff soil) [5], Fervers (highly accurate 2-D pneumatic tire model) [6], and Liu, et al (rigid wheel with critical state model of sand) [7]. Eventually Fervers applied his 2-D FEM realistic tire model to a range of simulated soil conditions [8]. Two-dimensional Discrete Element (DEM) models with rigid wheels were employed by Asaf, et al. (wheel driven by velocity boundary conditions, i.e. fixed slip) [9] and Li et al (particle shapes determined from lunar soil analysis) [10]. Even a coupled DEM/FEM
model was developed in 2-D by Nakashima and Takatsu, using a very stiff deformable tire and using velocity boundary conditions to specify its motion [11]. 3-D tire/terrain models were developed in FEM by Xia for frictional soil [12], and by Shoop, et al. for snow [13]. Hambleton performed finite element simulations comparing results of 2-D and 3-D models [14], [1], with results suggesting a strong presence of 3-D effects in the wheel/soil problem, and providing much of the inspiration for the DEM work done and for the future work proposed in this dissertation. Orr developed a 3-D FEM model of the Michelin Tweel®, tested it on a 3-D Drucker-Prager soil model with cap plasticity to simulate a nearly-non-cohesive lunar soil simulant, and produced results that also indicated extensive 3-D effects in the soil [2].

The current work has made steps toward continuance of Orr’s development of 3-D simulations by creating 2-D wheel/soil models in DEM that have paved the way for future 3-D models of the same. Further, the 2-D models in this work have been calibrated for shear strength using a statistical approach, which has not previously been done due to the computational effort required. These calibrated models have been tested with a variety of rigid wheel configurations to determine whether accurate estimates of traction and rolling resistance can be obtained from the 2-D models.
3. ABOUT DEM

The Discrete Element Method (DEM) is a numerical modeling technique that is not based on the assumption of continuous media. Instead a DEM model typically contains a collection of rigid bodies that interact with boundaries and with each other through contact. The deformation of a granular material such as sandy soil is almost completely due to the relative motion of whole grains instead of deformation within grains; therefore DEM is especially well-suited to modeling the behavior of these materials.

All DEM work in this study was performed in PFC2D (version 4.0), a two-dimensional DEM software package that is commercially available. A single license of the software was available; therefore work was limited to a single machine at any given time. This limitation prevented the use of a computing cluster. Also, version 4.0 of the code does not support parallel computing, so a multi-threading machine was not able to be fully utilized by the code. However, multiple sessions of PFC2D may be run at a time on the same machine; therefore, a multi-core machine may support up to the same number of separate PFC2D simulations as it has cores.

Because DEM uses explicit time integration, it is typically limited by processor speeds. Memory limitations are not generally a concern as they are in implicit integration methods. All the DEM simulation work in this study was performed on a Dell Precision T7400 workstation (Intel Xeon CPU E5420 @2.50 GHz x2, 8 GB RAM, 64-bit Windows operating system). Since each processor accommodates four threads, this machine was able to process up to eight single-thread DEM simulations simultaneously.
3.1. The algorithm

3.1.1. Contact Law

One of the most important parts of the DEM algorithm is its handling of contact. Contact is the main mechanism of particle interaction, and as such, is heavily responsible for the behavior of the DEM material as a whole. The most common contact model is represented graphically in Figure 3.1. The DEM code does not compute deformation of individual particles. Instead, the interaction between two particles is defined by a fictitious quantity called overlap. If the center points of two (round) particles become closer to each other than the sum of their respective radii, the particles are said to be overlapping. The value of the overlap ($\delta$) is calculated by Equation (3.1), in which $r_1$ and $r_2$ are the radii of the two particles in contact, and $d_{1\rightarrow2}$ is the distance between the two particle centers. As long as a negative value is computed by Equation (3.1), the overlap is taken to be zero. Although more complicated (and physically realistic) contact behavior can be incorporated into a simulation, the linear contact model, in which the normal component of the contact force is directly proportional to the degree of overlap, is the most common because of its minimal computational requirements. The spring constant governing normal forces in this model is referred to as the normal contact stiffness, and has units of force per unit length, as typical for a linear spring model. The tangential component of the contact force is determined in a similar way. Once contact is detected (i.e. overlap becomes non-zero), the code tracks the relative slip between the particles, using their radii and rotation angles. Again, the tangential component of the contact force is directly proportional to the relative slip, with the spring constant being
the so-called shear contact stiffness. Further, the shear force is not allowed to exceed the limit given by the product of the assigned friction coefficient and the current normal contact force. Finally, in order to dissipate energy from the system, the contacts include linear dashpots as well as springs. The dashpots provide forces contrary to the direction of relative velocity between two particles in proportion to their relative velocity. The dashpot forces are also added to the vector sum of the spring forces described earlier in this section, to determine the resultant contact force.

\[ \delta = (r_1 + r_2) - d_{1\rightarrow 2} \]  

(3.1)

![Figure 3.1: Particle contact (a), Normal contact model (b), Shear contact model (c)](image)

3.1.2. Calculation Cycle

The DEM calculation cycle consists of two main phases: the integration and the update. The integration phase begins knowing the acceleration and the initial velocity and position of each particle. The time integration is performed using an explicit scheme.
In order to maintain stability using explicit integration, the time increment must remain less than or equal to the maximum stable time step given in Equation (3.2), where $T$ is the smallest period of unforced oscillation in the system [15]. Instead of calculating the eigenvalues for the entire system, the frequency of each particle individually is calculated based on its mass and the stiffness of the contacts that it experiences at any given time. The particle with the highest frequency (and lowest period) is considered to provide a conservative estimate of the actual critical time increment. To further ensure stability, the calculated critical time increment is multiplied by a safety factor of 0.8, and this result is the time increment used in the code.

$$\Delta t_{crit} = \frac{T}{\pi} \quad (3.2)$$

Once the integration phase is complete, the code enters the update phase. During this phase the code searches for contacts (i.e. for the presence of overlap). A cell space search algorithm makes this process more efficient than a brute force approach would be, but still the search accounts for a significant portion of the computational effort in the method. Computational effort within the search algorithm is also the reason round particles are used: Locating the boundaries of round particles is simple compared to other geometries and it is important to minimize the computational requirements within the contact detection process. If purely circular particles do not adequately reproduce the behavior of the material in question, two or more circles may be clumped together into rigid clumps, allowing some control over shape without adding the computational burden of more complex geometries such as polygons or random shapes. Once the contacts have been identified, the contact law is used to compute the contact forces based on the new
positions of the particles. Finally, these forces and the moments they generate define particle accelerations (linear and angular) that will provide the starting point for the integration phase of the subsequent time increment.

### 3.1.3. 2-D modeling of 3-D particles

When considering the details of how certain 3-D physical phenomena are being approximated by a truly 2-D model, it is important to recognize that some interpretation is necessary. Technically, the 2-D DEM model is equivalent to neither a plane-strain nor a plane-stress situation for a 3-D material because neither motion nor forces are possible in the third dimension of the 2-D model; the third dimension simply does not exist in the model. However, since the plane-stress condition is uncommon in real life for frictional granular materials (the material would collapse without forces holding it together), the 2-D model probably can be thought of as plane-strain. Actually the 2-D model most closely resembles the cross-section of a collection of right cylinders stacked together, all having equal length, co-planar ends, and parallel axes. As such, ideally any input parameters of the model that pertain to the third spatial dimension should be handled by the software as normalized by length (e.g. mass per unit length would be computed as the product of density and area). This method of programming would result in a model that did not require the user to input the length of the cylinders, and for which the user would be required to scale his/her inputs according to the third-dimension of the problem.

PFC2D, however, does in fact require the third dimension’s length as an input called thickness, and assumes that all objects in the model have that thickness. The value is used for a single purpose: to compute the mass of each particle (as the product of density,
2-D area, and thickness). All quantities computed in the code are computed, not as distributed (per unit thickness), but as resultants. Quantities handled in this way include force, contact stiffness, and mass. Model values of these and other quantities must be divided by the thickness if this information is desired. For this reason, an incorrect thickness value in the model would effectively result in a mass-scaled problem that has altered inertial effects. Therefore the value of the thickness should be selected correctly to ensure that the mass of soil being disturbed by boundary conditions is correct. The thickness selection is particularly important for dynamic problems involving high acceleration of soil particles. Still, if for some unforeseen reason a PFC2D user strongly desired to scale the thickness to a value not corresponding to the appropriate dimension in the 3-D system, yet wished to avoid mass scaling and inaccurate particle accelerations, it is possible. The scaled thickness could be offset by scaling the material density input by the inverse factor, such that the product of the modified density and thickness is equal to the product of the original thickness and the actual material density. Any model having both thickness and density scaled in this way should produce identical results, regardless of the scale factor used.

3.2. Calibration of DEM Parameters

As with all simulation methods, the input parameters in a DEM simulation need to be calibrated to ensure that the material accurately demonstrates the physical characteristics important to the study. Traditionally this has been achieved through a trial-and-error approach in which the parameters are adjusted based on the outcome of previous simulations [16], [17]. Each iteration of trial and error requires at least one new
simulation to be computed. Although reasonable for quick-running simulations, this process quickly becomes infeasible as simulation run times increase, due the computational overhead involved. For example, a simulation of the direct shear test was used to calibrate the model to the strength properties of GRC-1 lunar soil simulant. The trial-and-error approach required 24 simulation cases, and the process required on the order of 12 weeks of computation on the Dell workstation. Further details on the direct shear test simulations are given in Chapter 4.

3.3. Creating Models of Test Specimens in DEM

3.3.1. Particle Number and Size

Much of the DEM modeling reported herein involves creation of models of physical tests so that the results can be compared to the actual physical experimental results. In the coming sections and chapters, the word “specimen” will refer to either a physical test specimen or a collection of particles that is being modeled, whichever is appropriate. Preparing a model of a physical test specimen of particulate matter using DEM (and specifically, PFC2D) is a non-trivial task. In some cases the preparation process may require more computational effort than is required by the virtual experiment itself that the specimen was created to accommodate. Preparing a static specimen requires several dynamic steps. First, a container must be defined, usually according to the geometry of the containing apparatus that is being simulated (shear box or sand trough, for example). The PFC2D software places a limiting condition of the generation of particles such that no particle may be created of size and location such that it will be initially in contact with another particle. One method that can be used to work around
this limitation is to generate particles in a larger container than actually needs filling. This way, all the particles fit with significant space separating them. The specimen is then compacted into the desired size and shape by moving the container’s boundaries. However this method was found to require excessive computational effort. A faster approach is to generate particles having a significantly smaller radius than will be required to fill the desired volume, allowing the randomly-generated particle positions to meet the restriction. Once created, the particles’ sizes may be arbitrarily increased until the desired volume is filled. This expansion causes significant interference between neighboring particles, and therefore large forces and violent motion subsequently. To reduce the violence of the response it is advisable to increase the particle sizes in small increments and to allow the code to cycle in between increases, relieving some of the unbalanced forces.

Even when increasing sizes gradually, particles may experience high velocities and may even escape through the walls of the container (by travelling further in a time increment than the length of one’s radius). If a particle escapes it will cause the cell space for the contact search algorithm to be expanded so that the stray particle remains within the cell space. As the particle drifts further and further from the main body of particles, expanding the cell space as it goes, the contact search algorithm becomes increasingly wasteful of resources and the code slows down significantly. To avoid this problem a custom algorithm is employed to automatically find and delete particles that have escaped the boundaries of the container.
Because of the restriction imposed on the particle generation process, it is necessary to know both the desired number of particles and the range of particle radius values in advance. That is, one cannot simply continue generating particles at the desired size until the volume is filled; the appropriate number of particles must be generated smaller than desired, and then expanded to the desired size. Therefore, Equation (3.3) was developed to estimate the radius limits that will result in a full volume for a given number of particles (see Appendix A for derivation). Equation (3.3) can be rearranged to solve for the number required if the user desires to specify size constraints instead of number. The equation was derived based on a uniform probability density of radius between upper and lower limits, where \( A \) is the domain area to be filled, \( r_{\text{min}} \) is the minimum radius permitted, \( \eta_{\text{target}} \) is the desired porosity of the specimen, \( F \) is the ratio of maximum radius permitted to minimum radius permitted, and \( n_{\text{balls}} \) is the number of particles to be created. In this research, Equation (3.3) was used to determine the final values in the specimen for minimum radius \( (r_{\text{min}}) \) and maximum radius \( (r_{\text{max}} = Fr_{\text{min}}) \), based on the number of particles desired. These desired values were divided by 16 to obtain values for the generation process; the radii were successively expanded and cycled as described above until they reached the desired values originally given by Equation (3.3).

\[
r_{\text{min}} = \sqrt[3]{\frac{3A(1 - \eta_{\text{target}})(F - 1)}{\pi n_{\text{balls}}(F^3 - 1)}}
\] (3.3)
3.3.2. **Porosity**

The final porosity (i.e. bulk density) of a specimen prior to testing is paramount to the behavior of the specimen. In physical experiments, a variety of techniques are employed to increase the density, including tamping and vibrating. Both these methods were attempted in simulation, with fair results in terms of their ability to compact specimens. However, both methods required an inordinate amount of computational effort and thus were abandoned. Instead, a non-physical method was developed to accurately achieve the needed porosity at a more manageable cost. The method begins with the particles as frictionless bodies. After expansion to the appropriate size as described above, with a target porosity somewhat higher than ultimately desired, one surface of the container is moved toward the specimen to increase its density. Because the particles are frictionless at this point, they readily rearrange themselves into a more compact configuration. Once the desired porosity is reached, friction is applied to the particles and the specimen is allowed to reach equilibrium.

3.3.3. **Equilibrium**

The final step of specimen preparation is allowing the particles sufficient time to settle to an equilibrium state. However any movement of any particle in the system will tend to cause adjacent particles to move, even though these movements become smaller and slower over time. There does not seem to be a straightforward way to consistently assess when the system has settled enough to be declared to be at equilibrium, so the answer to this question becomes a matter of judgment. Ideally, the system would reach a point beyond which further settling would result in no significant change in final outcome.
after the test has been completed. For example, if a specimen were truly in static equilibrium prior to performing a test on it, the outcome of the test would be the same whether performed immediately or an hour later, since the specimen would not have changed during that hour. Although this theory cannot be tested in the lab (since a physical test changes the specimen), it can be tested in simulation by saving the near-equilibrium state of the model prior to testing. Then the saved state can be restored and allowed to cycle through a given amount of simulated time (in which supposedly nothing is happening, if the specimen were originally at equilibrium), and then the test may be performed again. The results of the two tests can be compared, and would be expected to be identical if the system had been truly at equilibrium but to be slightly different if equilibrium was not quite reached prior to the testing.

This process was explored in depth, with many repetitions of saving, testing, settling further and re-testing, etc. It was found that for all but the simplest systems (<1000 particles) no point was able to be reached beyond which further settling had no effect on the test results. The plots in Figure 3.2 and Figure 3.3 illustrate this point. Each plot in Figure 3.2 is a stress-displacement curve for a different instance the same 1000-particle specimen, but each instance was allowed a different amount of time to settle. Each instance was settled for the base value of 960 milliseconds (selected by using the Average Unbalanced Force metric built into the code), plus the amount of time indicated in the text box on the plot. By inspection, the differences between the curves in Figure 3.2 are miniscule, and occur almost exclusively at high values of shear displacement (i.e. gross deformation). By contrast, the plots in Figure 3.3 were taken from multiple
instances of the same 6000-particle specimen (base settling time of 622 milliseconds),
and the differences are much more obvious. Still, however, the differences appear almost
exclusively after the first peak, that is, after the point when the particles’ displacements
become excessive.

Figure 3.2: Stress-displacement curves of different instances of the same 1000-grain
specimen sheared in a direct shear test after different durations of time allowed for
settling.
However, the variations caused by additional settling were not excessive in the sense that they did not result in significantly different final results. Also the variations due to extra settling were comparable to the variations observed when testing altogether different, randomly-generated specimens. It was concluded that allowing excessive amounts of time for settling was a waste of resources and did not achieve the desired effect. Therefore the question of equilibrium remains a judgment of the researcher. In this work, several metrics have been investigated for making this decision, including
velocity of the particles, kinetic energy in the system, and unbalanced forces in the system. None have been found to be consistently better than the others, so ultimately the average unbalanced force among the particles was used because the PFC2D code has a built-in tracking of this quantity. The proper threshold value for this metric depends on the parameters of the system, particularly the mass of the particles and the magnitude of static forces in the system; however for the direct shear test calibrations (Chapter 4) in this work a value of $5 \times 10^{-6}$ N was chosen. Once the simulation had experienced a value of average unbalanced force less than this threshold during a total of 1000 time increments, equilibrium was assumed to exist and the simulation proceeded to the next phase. During the calibration data collection, it was decided that the chosen value was too strict and resulted in excessive settling time in some cases; therefore for the rigid wheel experiments (Chapter 5) the value was revised to $1 \times 10^{-3}$ N.
4. DIRECT SHEAR TEST

The Direct Shear Test (DST) is a standard method used in geotechnical engineering to measure the shear strength of soil, especially of sand. The test involves a soil specimen that is confined under a known, generally constant pressure. While that confining pressure continues to be controlled, the specimen is sheared approximately along a given plane defined by the testing apparatus. During the shear, data are collected of the shear force and the volume of the specimen, and these quantities are typically plotted as a function of shear displacement. The shear stress-vs.-displacement plot (see Figure 4.) is used to characterize the strength and the packing density of the specimen. Two key quantities are extracted from this plot: the peak shear stress value and the large-displacement average shear stress value ("residual stress") which often is smaller than the peak value. Geotechnical engineers are usually primarily interested in the peak value because most soil designs are intended never to experience large displacements; however, for the problem of wheels on sandy soil both values have physical significance and both have been given equal attention in this research. Specific to the wheel/soil problem, the peak stress is considered to correspond to the case where a wheel is being operated without slip, while the residual stress corresponds to operation of a wheel with excessive slip.

4.1. Physical DST

The primary DST apparatus is the shear box. The shear box consists of three rigid parts. The upper and a lower box halves are bolted together to form an open-top cavity where the specimen will be prepared. The box halves are designed to interface with each
other by a single plane of contact, such that when the bolts are removed they will slide relative to each other along the plane of contact. This plane passes through the prepared specimen also and therefore becomes the plane of shear during the experiment. Once the specimen is prepared, a ‘lid’ (loading plate) is placed on top. The three parts together fully enclose the soil specimen. Moreover, the loading plate interfaces with the top box half such that the plate may move freely up or down (friction assumed negligible), thus changing the volume of the cavity. This allows control of the force applied to the top surface even if the specimen undergoes volume change during shearing. The cavity may be either cylindrical (i.e. having a circular shear area) or square in shape; a 50mm x 50mm square (specimen height about 16mm) was chosen in this case for its ability to be better represented by a two-dimensional model than a cylinder would be. Once the shear box is assembled with a specimen inside, it is placed in the loading apparatus for testing. The Geojac loading apparatus is controlled by a personal computer, and consists of a pair of actuators and load cells: one pair for the vertical axis and one for the horizontal. The vertical actuator will apply and maintain a constant force (i.e. normal stress) to the top surface of the specimen via the loading plate, as described above. The friction between the upper and lower halves of the shear box is eliminated by using the box’s assembly bolts to lift the upper half to provide a slight clearance from the lower half (about 0.01 inch, or 1/5-turn on a ¼” 20-threads-per-inch-bolt). The associated misalignment of the halves and the resulting moment applied to the specimen during shear are considered negligible. Once the shear box assembly bolts are removed, the horizontal actuator will push the bottom box half at a constant speed while the top half and the loading plate hold
their horizontal positions. As the specimen shears, the horizontal load cell records the force (i.e. shear stress resultant) required to accomplish the shearing (Figure 4.1). The DST apparatus is pictured in Figure 4.2. For further details on exact requirements of the test, see ASTM D-3080-04. For further information about the testing process, see [18].

![Typical Stress-displacement curves for sand from physical DST](image)

Figure 4.1: Typical Stress-displacement curves for sand from physical DST. Three curves at each confining pressure: 75kPa (lowest curves), 150kPa (middle), and 300kPa (highest).
4.2. Simulated DST

The two-dimensional DST simulation was developed to reproduce the physical setup as accurately as possible. The specimen dimensions were 50mm x 16mm before consolidation. Each specimen was sheared through a large displacement of 10mm, at a rate of 10 mm/s. This rate is much higher than the 1200 mm/s used in the physical experiment, but was necessary due to computational expense. Experiments were conducted to indicate whether the change in shear rate seriously affected the indicated strength of the soil; these experiments are described later in this chapter. Each type of specimen was tested at confining pressures of 75, 150, and 300 kPa. Custom algorithms controlled the motion of the top surface, seeking to achieve the desired conditions at each phase in the simulation. The simulation consisted of two main phases: specimen preparation and testing. The specimen preparation phase followed the procedure.
described in Chapter 3 to fill the domain volume with the proper number and size of particles, and to attain the correct initial porosity. Then the testing phase, consistent with the physical experiment, involved the application of confining stress and subsequent shearing of the specimen. All PFC codes used to control the simulation in its entirety can be found in Appendix (a).

Two control algorithms controlled the motion of the top surface at different times during the simulation. Both algorithms operated by specifying the vertical velocity of the surface, as determined by conditions in the specimen. First, during the specimen preparation phase, the porosity controller sought to obtain a specified porosity, which would be the so-called “initial” porosity at the start of the testing phase. If the specimen was not porous enough (i.e. too dense), the top surface would move upward, allowing the specimen to expand; if the porosity were high, the top would move downward to compact the specimen. Once the testing phase commenced, the porosity controller was turned off and the pressure controller took over the motion of the top surface. The pressure controller adjusted the top surface velocity according to the total vertical force exerted on the top surface. If the force were too low, the top moved downward; if too high, upward. Both controllers operated using a similar logic. The controlling quantity (porosity or force, respectively) was constantly compared to the target value and this difference was monitored in three ways: current value, time rate of change (i.e. derivative), and time-accumulated discrepancy (i.e. integral). These three values were modified if necessary (e.g. by providing a maximum acceptable value) and were multiplied by scaling factors obtained by trial and error. Finally the three were added together to obtain the new
velocity of the wall. The actual PFC code used for these two control algorithms may be found in Appendix (a).

Once the code for the DST was completed, it was used to gather data that would enable the calibration of parameters controlling the behavior of the soil. Rather than seeking initially to converge upon the behavior of a specific type of sand, the study sought to investigate a wide range of parameters with the goal of accumulating data that would be able to guide the selection of parameters to simulate many different varieties of sandy soil. The data were gathered in two phases. The first phase involved establishing a reference case and then varying one soil parameter at a time, to learn its individual effect. The following paragraphs contain a discussion of each parameter and the different graphs obtained by varying it. Later in the chapter, explanation will be given of the second phase, the determination of a statistical model for the calibration data.

4.2.1. Variation of a single parameter at a time

Following are results from 23 different cases of system parameters (i.e. simulated soil types), each simulated nine times (three each three different normal stresses). Only one parameter was varied at a time, making it possible to compare each parameter’s effect to a reference. For the 207 total simulations, typical computational time ranged from about 8 hours to about 40 hours per simulation, depending on parameters and on random factors in the stochastic samples. Each plot in the following figures contains nine curves: Three low (corresponding to 75 kPa confining pressure), three medium (150 kPa), and three high (300 kPa). The three curves within each confining pressure group also differ from each other; this is because each curve was obtained by running the
simulation with a randomly-generated particle set. The particle-generation process introduces randomness in two ways: position and size. To generate particles, horizontal and vertical boundaries are specified, within which the particles will lie. The program randomly selects the location of each particle within these boundaries. Similarly, as each particle is generated, its size is randomly selected according to the specified probability distribution (in this study, uniform probability within specified limits). This process allows the creation of random specimens as would be encountered in samples of physical soil.

4.2.1.1. Coefficient of Friction

The primary mechanism of inter-particle shearing surface traction in the DEM model is Coulomb friction. Thus, each contact has a coefficient of friction associated with it. In this study, a single value of the coefficient was used throughout any given simulation (i.e. all contacts in a single simulation had the same value). The frictional force is calculated from kinematics using the shear contact stiffness parameter (discussed in a future section) except when the calculated value exceeds the friction limit (the product of the coefficient of friction and the current normal force at that contact). When the calculated value exceeds the friction limit, the frictional force is simply set to the friction limit. This process is repeated for each time increment. It is noted that with this approach, no distinction is made between the static and kinetic coefficients of friction; they are equal by default. Figure 4.3 includes the results of four cases in addition to the reference case, each having its own coefficient of friction.
Figure 4.3: Influence of coefficient of friction at particle contacts on soil shear strength. Note the similarity between $\mu=3$ and $\mu=10$, probably because particle rolling is the dominant mechanism of relative motion.
4.2.1.2. **Normal Contact Stiffness**

The contact forces between particles in the DEM model are calculated in two components, normal and tangential, which are then added as vectors to obtain the total contact force vector. Although the particles are rigid bodies in the sense that internal deformation is not computed, the contacts are modeled as so-called “soft” contacts. This means that the contacts give slightly in order to permit the particle centers to move closer to each other than the sum of the radii, resulting in a small space that is dual-occupied by both particles. The normal component of the contact force is estimated from this overlap using the parameter called normal contact stiffness. The normal force is equal to the product of the overlap distance and the normal contact stiffness parameter (units of force/length). In general the contacts may be assigned individual values but for this study, all contacts in a given simulation have the same contact stiffness. Figure 4.4 contains the results obtained by increasing this parameter. From the figure it is apparent that increased normal stiffness results in reaching the peak shear stress at a lower displacement. In addition, stiffer contacts resulted in slightly stronger peak strength but very similar residual strength. The increase in shear strength demonstrated by stiffer contacts is probably due to a greater volumetric dilation of the specimen since the grains do not “overlap” (penetrate into each other) as much. It is also noteworthy that higher stiffness values tend to result in much longer computational times since they require smaller time increments to be used.
4.2.1.3. *Shear Contact Stiffness*

The tangential component of the contact force is calculated in a manner similar to the normal component. When two particles come into contact, the shear force is set to zero and the point of initial contact is recorded for each body. As relative motion occurs (in the tangential direction) between the contact point on one body and the contact point on the other body, a slip distance is calculated. In essence the slip distance is equal to the tangential component of the distance separating the contact points of the two bodies, and is obtained from knowledge of the particle radii and rotations after contact formed. The tangential force component then is simply the product of the slip distance and the shear contact stiffness parameter (units of force/length), but cannot exceed the limiting value given by the friction limit. Like the normal stiffness, the shear stiffness may be defined separately for each contact, but in this study all contacts had the same value within a
given simulation. See Figure 4.5 for results of varying this parameter. It is important to note that higher stiffness values tend to result in much longer computational times.

![Figure 4.5](image)

Figure 4.5: Influence of shear contact stiffness (N/m) on soil shear strength.

An interaction between friction coefficient and shear contact stiffness in the development of shear stress within a specimen was suspected because of the role that both play in the computation of shear forces between particles. Specifically, it was supposed that if the average particle size were small enough, and if the shear stiffness were low enough, then two particles sliding across each other (in translation) would lose contact with each other before enough shear force could develop to exceed the friction limit. If this were the case, further increases in friction coefficient would have no effect, as is apparent when comparing friction coefficients of 3 and 10 in Figure 4.3. Also the value of friction coefficient at which further increases had no effect would be higher at higher shear stiffness levels. To test whether the lack of difference between the friction coefficients of 3 and 10 was due to this interaction, tests for the five friction values were
repeated at different shear stiffness levels. If the interaction were responsible for the strength similarities between friction coefficients 3 and 10 in Figure 4.3, it was expected, for example, to see similarity between coefficients 1, 3, and 10 when the shear stiffness was decreased. On the other hand, one would expect to see continued upward trend of strength with friction value (i.e. no limit in strength for increasing friction value) when the shear stiffness was increased. However, the plots in Figure 4.6 and Figure 4.7 demonstrate a similar trend as Figure 4.3. In all cases, there is increasing strength until the coefficient of friction reaches 3, at which point the strength levels off. Although the strengths for friction values of 3 and 10 are roughly the same as each other in every case of shear stiffness, they increase notably when the stiffness is higher; on the contrary the shear strength for lower values of friction does not change significantly with shear stiffness. Thus there appears to be a mild interaction between friction coefficient and shear strength, but it is not manifested in the way anticipated.
Figure 4.6: Coefficient of friction varied at lowered level of normal stiffness (Ks). Compare to Figure 4.7 and Figure 4.3.
Figure 4.7: Coefficient of friction varied at raised level of normal stiffness (Ks).
4.2.1.4. Eccentricity of Particle Shape

One of the most significant simplifying assumptions of the DEM model is that all particles are circular. This assumption is used because of the tremendous computational advantage it offers in terms of calculating where a particle’s boundaries are. While it is possible to significantly increase simulation accuracy by giving a polygonal or other shape to the particles at great computational expense, a compromising approach is to form non-circular particles by connecting multiple circular particles kinematically into a single rigid clump. A variety of shapes can be made using two particles per clump; far more options exist using three. For simplicity, this work uses two overlapping equal-radius particles per clump, referred to as dyads. The shape of the dyad is described by its eccentricity, or the number of particle radii separating the two circle centers. For example, an eccentricity of zero is simply a circle; an eccentricity of 2r places the particles tangent to each other; an eccentricity greater than 2r places the particles with a fixed distance between them. Figure 4.8 contains an illustration of each shape with its plot for clarity.
Figure 4.8: Six levels of dyad eccentricity. Increases in eccentricity result in large increases in both peak strength and residual strength.

4.2.1.5. Pre-confine ment packing density

The parameters discussed so far are variables in a DEM simulation but not in the physical experiment. That is, once a physical soil is selected, the contact friction, the stiffness, and the particle shape are inherent in that selection. Unlike those parameters, the initial packing density (i.e. porosity, the ratio of void volume to total volume) of a
physical specimen is a function of how the specimen is prepared in the lab. The packing density has a strong influence on the results of a soil strength test. If the initial packing density is above a certain level (the critical state), a very different behavior will be observed than if it is below the critical state level. Essentially, if the soil is denser than critical state, the specimen will expand during shear until it reaches critical state in the failure region, resulting in a peak shear strength that occurs early (low horizontal displacement), followed by a somewhat lower strength (residual strength) as the shear displacement becomes large. In this case the greater the initial density, the more distinct and the greater the peak strength. If the specimen is packed looser than critical state density, it will compress further during shear until it reaches critical state, resulting in a shear stress that builds slowly until it reaches and maintains the residual strength stress value. In this case there is no peak; the residual strength is also the maximum stress developed. The looser the specimen, the greater shear the displacement required to reach residual stress. It is important to note that the residual stress corresponds to shear at critical state density and will be roughly the same shear stress value regardless of the initial packing density. This study has focused on specimens prepared denser than critical state based on the assumption that soils in the field, if they have been undisturbed for a long time, will tend to have this characteristic. Thus the specimen preparation in the lab included efforts to pack the sand as densely as possible by manual tamping and manual shaking.

A variety of specimen preparation techniques were attempted for the simulations, including tamping and shaking. Although these methods were found able to make the
specimen denser than critical state, they required a great deal of additional simulation time. It was found that the particles would pack much more readily if friction was not activated in the simulation (i.e. if the coefficient of friction were zero). Using this method it was found possible to produce specimens much denser than could be produced in the lab, as evidenced by dramatic expansion and unusually high peak stresses during shear. Ultimately, the approach taken was to define a desired level of porosity (the input parameter), then gradually compress the specimen without friction until it reaches that level. Once stable in that state (i.e. the particles reach equilibrium), the friction is activated to hinder further packing, the confining pressure is applied, and the shearing is performed. This method of creating the desired pre-confinement density was able to control the behavior during shear, as evidenced by the curves in Figure 4.9.
Figure 4.9: Comparison of different pre-confinement packing states in terms of 2-D porosity. Note that a lower porosity corresponds to a higher packing density. Also note that the residual stress (stress value at large strains) is roughly the same for all cases.
4.2.1.6. Rate of Shear

The details of the simulation for the direct shear test were designed according to the ASTM standard for direct shear test of sands (ASTM D3080-04). The standard specifies a technique for selecting the proper shear rate, depending on the hydraulic conductivity of the sample. A typical value for shear rate for a dry sand is 0.0125 inch/min (1/4 inch in 20 minutes). Unfortunately such a shear rate is not feasible for the DEM model used in this study because one simulation would require over a year of wall time. Since the sand in this study is dry (no water drainage effects), a faster shear rate will not introduce inaccuracy due to hydraulic effects. However, for calibration purposes, it is important that the rate not be so high as to introduce inaccuracy due to inertial effects that are not present in the extremely slow physical experiment. The shear rate of 1 cm/sec (23.6 inch/min) was arbitrarily selected. The results shown in Figure 4.10 demonstrate that changes in shear rate around this value do not produce a significant change in the predicted strength, and therefore suggest that particle inertia is not a significant source of inaccuracy at this rate.
Figure 4.10: Stress-displacement curves for different shear rates. The agreement between the curves is interpreted as an indication that the inertia effects are not significant for rates around 1 cm/s.

4.2.1.7. Upscale Factor

The influence of upscale factor on the results of a simulation is important to consider because of the computational limitations of DEM. Since computational resources place a practical limit on the number of elements available for a DEM simulation, the size of the particles in the simulation must be scaled large enough that the available number of particles will fill the needed volume. A way has not yet been found to avoid this simplification, thus simulations have been performed at different levels of scaling in order to demonstrate that results of scaled simulations are reasonable. Results from different levels of upscale are shown below in Figure 4.11. In the figure it is apparent that as upscale increases, measured strengths increase. This observation is characteristic of what would be expected when increasing inertia in the system. Also the curves became noticeably simpler when the upscale reached a value of ten. This is because a data point was recorded after a given number of time increments; fewer
increments were required in the upscaled system and thus fewer data points were recorded.

Figure 4.11: Results from different system scale factors. Note that horizontal scales are different.

Nearly every input relating to length in the system was scaled by the same factor, including box dimensions, particle diameter, rate of shear, and stress (force per unit length in 2-D). The only inputs that were not scaled are the shear and normal stiffness parameters. This decision was made in the interest of maintaining comparable overlap at the contacts between simulations of different scaling. In a larger-scaled simulation, a typical contact will transfer a proportionally greater force than a typical contact in a smaller-scaled simulation, resulting in a proportionally greater overlap distance (with the same stiffness value). However, the diameter of the particles is also proportionally larger. Thus, considering the overlap relative to the diameter (i.e. a unitless ratio of lengths), this situation results in a relative overlap that is comparable between the two simulations.
A potential source of inaccuracy in the scaled DST simulation arises from the fact that a particle comes to represent a group of grains. This means that although the inertial resistance to translation (i.e. the mass of the group of grains) is reasonably approximated, there is the potential for a significant increase in resistance to shear forces because the rotational inertia is significantly higher for the large particle due to its larger radius. That is, much more effort would be required to cause rigid-body-like rotation of a group of grains (as represented by one large, scaled particle) than would be required to cause each particle to rotate about its own center. For this reason, whereas small particles may provide comparatively little resistance to shear (by easily beginning to roll), scaled-up particles may develop unrealistically high resistance to transient shear loads; this problem is exacerbated by the fact that the velocity of the shear box increases with scale and thus the problem is all the more severely transient. An inadvertent advantage of this increase of inertia is an increase in stable time increment for the explicit integration algorithm. Since the moment of inertia is greater but shear stiffness is constant, the natural frequencies are lower and the stable time increment is larger; thus fewer increments are needed to simulate a given time interval. This fact can be exploited by scaling strictly for computational advantage, but such should be done only with great caution because of the potential for sacrificing accuracy due to the reasons discussed.

A different approach to upscaling is to avoid scaling the shear rate. This would result in longer simulated times but would require comparable wall times as the unscaled simulations since the time step would be larger. It could also help alleviate some of the inaccuracy due to higher particle inertia since the box velocity (and corresponding
particle velocities and accelerations) would not be increased with problem scale. Yet another possibility for particle scaling is to scale the particles without scaling the whole system, thus reducing the total number of particles needed to fill the system and drastically reducing the degrees of freedom in the system and the computational expense of the simulation. This approach will be used for wheel/soil models in a later chapter.

4.2.2. Calibration by trial and error

The simulation data that have been discussed to this point included the first 24 cases listed in Table 4.2, and each of these cases examined the effect of a single variable on shear strength. These data were gathered and analyzed qualitatively as described in the preceding paragraphs. Such a qualitative analysis is helpful for understanding the individual effects of the parameters on shear strength; that information can then be used to guide the direction of parameter adjustment during the traditional, trial-and-error based calibration process (see also [19]). Cases 25 through 47 in the table represent the iterations of the trial-and-error process seeking to match the strength of GRC-1. Case 47 produced the closest match to the physical experiment and was taken as the appropriate set of parameters for simulations involving the strength of GRC-1; the stress-displacement plots are displayed in Figure 4.12.
4.2.3. Calibration by statistical model

A qualitative understanding of the effect of parameters was obtained by altering a single variable at a time. Although this knowledge can guide the quantitative selection of parameters for calibration using trial and error, it would be more useful to produce a method that can directly specify an appropriate set of parameters for the strength desired. Also, it was recognized that independent treatment of variables was not adequate because some interactions between parameters may exist. Therefore the goals of developing an explicit quantitative model and of identifying potential interactions (especially between friction coefficient, eccentricity, and shear stiffness), were added to the scope of the calibration study. The goals were achieved through the creation of statistical models to predict the maximum and minimum bulk density, the shear strength (peak and residual),

Figure 4.12: Stress-displacement curves for GRC-1 from physical DST (left), and calibrated DST simulation (right).
and the initial (i.e. small-displacement) shear stiffness of a DEM specimen based on the input parameters.

4.2.3.1. Statistical Models

A linear least-squares regression algorithm was used to develop all the statistical models in this work. It is important to note that a linear statistical model may include nonlinear relationships between any factor and the outcome by transforming a factor into a “new” variable; the term linear merely denotes first-order proportionality between the transformed variables and the outcome. For example, the following relationship is clearly linear and could be obtained from a linear least-squares regression:

\[ y = 4.22x + 2.33t \]  (4.1)

However, if the user has created the variable \( t \) through the transformation \( t = x^2 \), then the user recognizes the model to represent a nonlinear relationship, even though the algorithm developing the model was not “aware” of this fact:

\[ y = 4.22x + 2.33x^2 \]  (4.2)

In this way a linear regression model may include nonlinear relationships between the factors and the outcome.

4.2.3.2. Relative Density

During analysis of the DST data it was observed that, for a given value of porosity, some parameter combinations produced the characteristic stress-displacement curve of a loosely packed sand, while other combinations behaved as a densely-packed sand. A similar situation is observed in different types of physical sand also, in which the distinction between a “loose” sand and a “dense” sand is defined not in terms of absolute
packing density but in terms of the so-called relative density of the specimen. The relative density is given by equation (4.3), in which \( D_R \) is the relative density, \( e_{\text{min}} \) is the minimum possible void ratio of the soil type (i.e. the densest state), \( e_{\text{max}} \) is the maximum void ratio (the loosest state), and \( e_{\text{cur}} \) is the current void ratio of the specimen or the void ratio in question:

\[
D_R = \frac{e_{\text{MAX}} - e_{\text{CUR}}}{e_{\text{MAX}} - e_{\text{MIN}}} \tag{4.3}
\]

It is apparent from Equation (4.3) that a relative density of zero corresponds to the loosest state for that soil type. Similarly, a relative density of unity corresponds to the densest state possible for that soil type. Typically, a sand specimen prepared below a relative density of 0.5 is considered “loose” while a specimen prepared with a relative density above 0.7 is “dense” [18]. It is important to note that Equation (4.3) contains void ratio values, while the DEM data are reported in porosity. Therefore conversion must be made in order to use Equation (4.3) with the DEM data. The relationship between void ratio (VR) and porosity (\( n \)) is:

\[
n = \frac{VR}{1 + VR} \tag{4.4}
\]

To compute the relative density of a DEM specimen knowing the specimen porosity, it was necessary to determine the minimum and maximum possible void ratio levels for that specimen’s parameter set. A simulated experiment was developed to measure these values for a particular DEM specimen. The relative density simulation consisted of a box with a movable top surface like the direct shear box. The specimen was created to fill the box as described in Chapter 3. However instead of using the top of
the box to compact the frictionless particles to a target porosity, the top of the box remained stationary. The particles’ friction was enabled, gravity was enabled, and the particles fell (“snowed”) to the bottom of the box. Once the specimen reached equilibrium, the porosity was measured throughout the specimen and was taken to be the loosest possible configuration of that specimen type ($VR_{MAX}$). It is noted that a great deal of computational effort was required to reach the equilibrium point under these conditions. Once done, the particles’ friction was disabled, the top of the box descended to apply a confining pressure of 75kPa. Then the top of the box was slowly raised until it lost contact with the particles, and the particles were again allowed to reach equilibrium. This equilibrium point was taken as the densest possible unconfined state for that specimen type ($VR_{MIN}$). This experiment was conducted over a range of values for friction coefficient, eccentricity, and normal stiffness; these were considered to be the parameters that might influence the porosity limits. Table 4.1 contains the parameter combinations and results from this set of simulations.

Table 4.1: Input parameters for the data set used to determine relative density (26 simulations total)

<table>
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<tr>
<th>Case number</th>
<th>Friction Coefficient</th>
<th>Dyad Eccentricity</th>
<th>Normal Stiffness</th>
<th>Quantity Simulated</th>
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The results from the simulations defined in Table 4.1 were used to develop a pair of statistical models that predict the minimum and maximum density of a DEM soil, based on the input parameters. These values would be used to define the relative density of a given specimen. Maximum density (i.e. minimum porosity) was modeled first. The first step in the statistical modeling process was to generate an all-inclusive model including terms for all factors, transformed factors, and interactions of factors considered likely to be significant. This initial model provided information about what factors and interactions actually belong in the final model, that is, which ones were actually useful in predicting the outcome. The regression yielded the following equation, where $n_{\text{min}}$ is minimum relative density, $e$ is dyad eccentricity, $\mu$ is friction coefficient, $Kn$ is normal contact stiffness:

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\[ n_{\text{min}} = 0.1488 + 7.195E(-5)\mu - 6.037E(-5)\ln(\mu) - 9.467E(-2)e \\
+ 4.910E(-2)e^2 + 2.693E(-11)K_n \] (4.5)

The statistical software provides standard metrics to evaluate how well the model fits the data supplied. One such metric, the correlation coefficient (or “R\(^2\) value”), represents the percentage of the variation in the outcome variable that is explained by the model. The R\(^2\) value for this all-inclusive model was .9997, meaning that 99.97% of the variation in minimum porosity is explained by the model. Besides the R\(^2\) value, the software provides p-value metrics, which indicate the significance of each term in the model. A low p-value indicates a high probability of significance. As expected, some of the terms do not add significant predictive value to the model. Every factor with a p-value greater than 0.1 was discarded. The model was then recomputed with the remaining factors to obtain:

\[ n_{\text{min}} = 0.1491 - 9.480E(-2)e + 4.915E(-2)e^2 + 2.693E(-11)K_n \] (4.6)

This model still had an R\(^2\) value of 0.9997. The p-value for the \(K_n\) term was eight orders of magnitude higher than for the other terms, so a final model was generated excluding the effect of \(K_n\):

\[ n_{\text{min}} = 0.1505 - 9.480E(-2)e + 4.915E(-2)e^2 \] (4.7)

The R\(^2\) value for the final model was 0.9988, indicating that over 99% of the variation of minimum porosity is explained by Equation (4.7), which is dependent solely on grain shape. This is not surprising since common experience would suggest that the densest
packing arrangement of a collection of objects in general depends almost exclusively on their shape.

The minimum density (i.e. maximum porosity) of a specimen was modeled using a similar process as the maximum density. For an all-inclusive model, the data yielded the following equation, where $n_{\text{max}}$ is maximum relative density, $e$ is dyad eccentricity, $\mu$ is friction coefficient, $Kn$ is normal contact stiffness:

$$n_{\text{max}} = 0.2210 - 5.676E(-3)\mu + 3.081E(-2) \ln(\mu) - 5.878E(-2)e$$

$$+ 4.259E(-2)e^2 - 4.048E(-11)Kn$$  \hspace{1cm} (4.8)

This all-inclusive model had a correlation coefficient of 0.9628. Eliminating terms with a p-value greater than 0.1, the model is:

$$n_{\text{max}} = 0.2188 - 5.676E(-3)\mu + 3.081E(-2) \ln(\mu) - 5.878E(-2)e$$

$$+ 4.259E(-2)e^2$$  \hspace{1cm} (4.9)

This model had no significant loss in correlation; the coefficient was 0.9619. After further selecting factors to eliminate from the model according to highest remaining p-value, the final model is:

$$n_{\text{max}} = 0.1799 + 1.942E(-2) \ln(\mu) + 2.056E(-2)e^2$$  \hspace{1cm} (4.10)

The $R^2$ value for this final model of maximum porosity as a function of friction coefficient and dyad eccentricity was 0.8846 (88% of variation in maximum porosity values explained by the model).
4.2.3.3.  **DST simulation cases**

The remaining statistical models estimate shear strength and shear stiffness properties of DEM specimens, based on simulation input parameters. The models were computed using all the data from the single-factor part of the calibration study, mentioned earlier in this chapter, except for the cases examining shear rate or upscale factor. In addition to the single-factor simulations, a number of simulations were conducted while varying more than one simulation parameter at a time; these simulations were selected for the purpose of helping to identify possible interactions between certain factors. The results from the multiple-factor simulations were also included in the statistical model computations for shear strength and stiffness properties. Table 4.2 contains the complete set of parameter combinations used to generate the data for the subsequent models.

Table 4.2: Input parameters for the entire data set of direct shear test (364 DST simulations total)

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<th>Normal Stiffness$^2$</th>
<th>Shear Stiffness$^2$</th>
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The next property of interest was friction angle for residual stress. Residual stress is the ‘steady-state’ value of shear stress as shear displacement becomes large. This property of soil is relevant to the problem of a wheel operating on sandy soil because in situations where the wheel spins/slips on the soil, a large shear displacement is expected. The friction angle of residual stress was computed from the stress-displacement curve of each simulation. For each simulation’s curve, a custom algorithm determined the shear displacement where the stress reached its maximum value. Based on that displacement, the algorithm decided whether the specimen was demonstrating loose behavior or dense,
and this decision determined the value of displacement at which steady-state stress was
assumed to have been reached. The mean stress was computed starting from this
displacement until the end of the simulation, and was taken to be the residual stress for
the simulation.

Similar to the minimum and maximum density models, the first step was to
generate an all-inclusive model including terms for all factors, transformed factors, and
interactions of factors considered likely to be significant. Since there were far more data
points for strength than for minimum and maximum porosity, and since the number of
parameters thought likely to contribute was greater, the all-inclusive model had a great
many terms. The regression yielded the following equation, where $\phi_R$ is friction angle
for residual stress, $e$ is dyad eccentricity, $\mu$ is friction coefficient, $Kn$ is normal contact
stiffness, $Ks$ is shear contact stiffness, and $n$ is pre-confinement specimen porosity:

$$
\phi_R = -1.052E5 + 5.679e - 0.7189e^2 + 0.4348 \exp(e) - 11.04\mu \\
+ 1.895\mu^2 + 6.710 \ln(\mu) - 4.673E(-3) \exp(\mu) \\
+ 7.403E(-9)Kn - 4.243E(-18)Kn^2 \\
- 3.441E(-9)Ks + 1.612E(-18)Ks^2 \\
+ 0.5467 \ln(Ks) - 9.672E4n - 6.912E4n^2 \\
- 443.8 \ln(n) + 1.036E5exp(n) - .1660e\mu \\
+ 1.929E(-10)\mu Ks
$$

(4.11)

The correlation coefficient for this all-inclusive model was .9059, meaning that 90.59%
of the variation in residual friction angle is explained by the model. As expected, many
of the terms do not add significant predictive value to the model, based on the p-value
metric. Every factor with a p-value greater than 0.1 was discarded. The model was then
recomputed with the remaining factors to obtain:
\[
\phi_R = 26.11 + 5.623e - 9.782\mu + 1.597\mu^2 + 6.462 \ln(\mu) \\
- .0038 \exp(\mu) + 0.2534 \ln(Ks) - 0.1625e\mu
\] (4.12)

The R\(^2\) value for this model was .9000, almost as high as for the all-inclusive model. Again, the p-values for all the terms were considered, and it was observed that two of the factors had significantly lower p-values than all the others. So, these two factors were retained and the others dropped:

\[
\phi_R = 21.80 + 5.517e + 1.328 \ln(\mu)
\] (4.13)

This equation still had an R\(^2\) value of .8304, meaning that 83.04\% of the variation in residual friction angle was explained by the equation; this equation was taken as the final model for use in subsequent computations.

4.2.3.5. Friction Angle of Peak Stress

Next, a model was developed to predict the friction angle of peak stress. Peak stress for each simulation was taken simply as the maximum stress value obtained for each stress-displacement curve. Rather than model this quantity from the base parameters, the model was developed to provide a relationship between the friction angle of residual stress and the relative density. This approach was taken for two reasons. First, physical sand tests demonstrate dependence of peak stress on little besides residual stress and specimen preparation. Second, this approach would lead to a unique choice of model parameters to produce a desired residual stress and peak stress. On the other hand, if the friction angle for peak stress were modeled as an explicit function of friction coefficient, dyad eccentricity, etc., the resulting model would in all likelihood conflict with Equation (4.13) such that both desired friction angles could not be obtained through
a single parameter set. Modeling peak stress as a function of residual stress, however, allows for the selection of friction coefficient and dyad eccentricity by Equation (4.13) to produce the desired residual stress, and then subsequently for the selection of relative density (i.e. the input parameter of porosity) to control the peak stress. Three terms were included in the initial model, where $\phi_p$ is friction angle for peak stress, $\phi_r$ is friction angle for residual stress, and $D_R$ is the relative density:

$$\phi_p = 11.73 + 0.5565\phi_r - 23.13D_R + 1.581\phi_r D_R$$  

(4.14)

This model had a correlation coefficient of 0.7596. The p-value metric indicated the residual friction angle to be the least value-adding factor in the model, it was judged important to retain its presence because of the well-accepted correspondence between peak and residual stresses in physical systems [18] Therefore the linear term for relative density (having the next-highest p-value) was removed instead, with good results:

$$\phi_p = -7.359 + 1.236\phi_r + 0.7495\phi_r D_R$$  

(4.15)

Equation (4.15) demonstrated little change in correlation as compared to Equation (4.14): $R^2 = 0.7485$. Further, both factors were now assigned very low p-values, indicating significant value added to the model by each. Equation (4.15) was accepted as the final model to be used in parameter selection for friction angle of peak stress.

4.2.3.6. Shear Stiffness

Finally, the initial shear stiffness of a specimen was investigated with the goal of modeling it in a similar fashion. For each simulation, the shear stiffness was computed from the stress-displacement curve. Two points on the curve were identified: the point at
which the stress reached 10% of the peak value, and the point at which the stressed reached 80% of peak. The difference in stress values was divided by the difference in the displacement values at which those stress values was reached, with this ratio being taken as the initial slope, i.e. the average slope during the phase of rapidly increasing stress before significant grain slippage began.

Like residual friction angle, stiffness was modeled from the base parameters, because it was not of key importance to predict shear stiffness simultaneously with shear strength, and because it was anticipated that different parameters would be of primary influence for stiffness than for strength. The initial, all-inclusive model was computed as follows, where $G$ is the shear stiffness, $e$ is dyad eccentricity, $\mu$ is friction coefficient, $Kn$ is normal contact stiffness, $Ks$ is shear contact stiffness, $n$ is pre-confinement specimen porosity, and $\sigma_n$ is applied normal stress:

\[
G = -5.058E(13) - 3.447E(8)e + 1.839E(7)e^2 + 1.129E(8)\exp(e) \\
- 2.437E(8)\mu + 4.427E(7)\mu^2 + 1.938E(8)\ln(\mu) \\
- 1.214E(5)\exp(\mu) + 1.602Kn - 3.497E(-10)Kn^2 \\
+ 1.780E(-1)Ks - 2.382E(-10)Ks^2 + 4.454E(7)\ln(Ks) \\
- 4.629E(13)n - 3.336E(13)n^2 - 2.329E(11)\ln(n) \\
+ 4.978E(13)\exp(n) - 4.866E(1)\sigma_n + 1.401E(8)\ln(\sigma_n) \\
+ 9.811E(6)e\mu + 4.122E(-2)\mu Ks
\] (4.16)

The correlation coefficient for the above model was 0.8009. Factors with a p-value greater than 0.1 were dropped, leaving the following:

\[
G = -4.985E(13) - 3.339E(8)e + 1.219E(8)\exp(e) - 3.113E(7)\mu \\
+ 1.270E(8)\ln(\mu) + 1.227Kn + 5.399E(7)\ln(Ks) \\
- 4.561E(13)n - 3.289E(13)n^2 - 2.309E(11)\ln(n) \\
+ 4.905E(13)\exp(n) + 1.335E(8)\ln(\sigma_n) \\
+ 9.443E(6)e\mu
\] (4.17)
The new correlation coefficient was hardly changed, with the value now being 0.7971. As done previously, the model was further simplified by eliminating all but the very lowest p-values: all factors with a p-value greater than 2E-16 were taken out to produce the final model for initial shear stiffness:

\[
G = -1.340E(9) - 3.572E(8)e + 1.198E(8) \exp(e) \\
+ 9.243E(7) \ln(\mu) + 1.300Kn + 1.146E(8) \ln(\sigma_n) \tag{4.18}
\]

Although care was taken to retain factors in the model that had the greatest significance according to the statistical metric, the final model had a notably lower correlation coefficient than did its predecessor: the value had now dropped to 0.6134. Because the iterations of the shear stiffness model have demonstrated this behavior in which even many of the less significant factors apparently contribute to the accuracy of the model, it is suspected that there is a problem with either the modeling process or the stiffness data. A possible issue with the modeling process would be the failure to include one or more key factors in the all-inclusive model for shear stiffness. More likely, however, it seems that the values themselves may not be sufficiently accurate because of the way the stiffness of each sample was computed: in most cases the slope was determined from a small number of data points (between 2 and 10) from the stress-displacement curve. These data were recorded during the phase of the direct shear test that is the most sensitive to changing displacement and arguably would have benefitted from a higher sampling rate. For this reason, little confidence is placed in the validity of the above models for shear stiffness; yet if one must be used, of the equations presented, Equation (4.17) probably offers the best balance between simplicity and accuracy.
4.2.3.7. Using Statistical Models to Select Simulation Parameters for Desired Friction Angles (Peak and Residual)

The purpose of the statistical models developed in the preceding pages was to expedite the process of calibration a DEM simulation to a specific type of sand. Rather than use a trial-and-error approach as described previously, a direct approach was desired and was sought through the statistical models. Such an approach has been realized by means of the equations above, and for the single test case attempted, has provided acceptable results.

The sand used in the test case was a typical silica sand. The sand could be described as feeling similar to the sand one might expect to find on a sand volleyball court, i.e., the sand is soft and of moderately small grain size (estimated typical diameter 0.05-0.5 mm). The sand was selected because it was the current medium contained in the Merry-Go-Round wheel testing system, to be described in a subsequent chapter; the sand is subsequently referred to as “MGR sand”. In order to select a set of DEM simulation parameters that reproduces the strength behavior of the MGR sand, three direct shear tests were performed on a sample of the sand. The stress-displacement curves for MGR sand are displayed in Figure 4.13.
Figure 4.13: Stress-Displacement curves for DST of MGR sand (left); and envelope plots for peak and residual stress of MGR sand (right).

The envelopes in Figure 4.13 indicate a peak friction angle of 39.0° and a residual friction angle of 32.5°. Using this friction angle for residual stress in conjunction with Equation (4.13), a relationship was developed between coefficient of friction and particle eccentricity:

\[
32.5 = 21.80 + 5.517e + 1.328 \ln(\mu) \rightarrow \\
\frac{e = \frac{32.5 - 21.8 - 1.328 \ln(\mu)}{5.517}}{(4.19)}
\]

Equation (4.19) is plotted in Figure 4.14.
Figure 4.14: Plot of Equation (4.19). Points on the curve represent parameter combinations that are expected to reproduce the residual stress friction angle of MGR sand.

Any pair of values that satisfies this relationship (in the range of the data used to generate the model) is expected to result in a sand model that has residual stress of MGR sand. Two arbitrary pairs were selected to use in validation: pair 1) $\mu = 0.7$, $e = 2.02$ and pair 2) $\mu = 2$, $e = 1.77$.

Knowing both friction angles (for peak and residual stresses) of the desired sand, Equation (4.15) was used to estimate the target relative density in the simulation:

$$39 = -7.359 + 1.236(32.5) + 0.7495(32.5)D_R \Rightarrow D_R = 0.25$$  (4.20)
Having selected two friction/eccentricity pairs of interest, Equations (4.7) and (4.10), respectively, were used to estimate the minimum porosity and the maximum porosity possible for each case. Case 1 resulted in a maximum porosity of 0.257 and a minimum of 0.160, while Case 2 yielded a maximum of 0.258 and a minimum of 0.137. These estimates of the minimum and maximum porosity were converted to void ratio by Equation (4.4), then were used along with the target relative density prescribed by Equation (4.20) to specify the target void ratio through Equation (4.3). Finally Equation (4.4) was used again to convert the target void ratio back to the required simulation input parameter of porosity. This series of steps resulted in the following values for target specimen porosity: case 1) \( n = 0.235 \) and case 2) \( n = 0.231 \).

The steps described in the preceding paragraphs use the statistical model equations to select appropriate simulation parameters based on desired peak stress and residual stress friction angles. The process is summarized with key values in Table 4.3.
Table 4.3: Steps of the parameter-selection process using statistical model, with resulting values of two possible parameter sets for MGR sand.

<table>
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<tr>
<th>Step</th>
<th>Input(s)</th>
<th>case 1 input values</th>
<th>case 2 input values</th>
<th>Equation(s)</th>
<th>Output(s)</th>
<th>case 1 output values</th>
<th>case 2 output values</th>
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<td>$\phi_r$ (from lab), $\mu$ (arbitrary)</td>
<td>32.5°, 0.7</td>
<td>32.5°, 2.0</td>
<td>4.13</td>
<td>Figure 14, $e$</td>
<td>$e = 2.02$ radii</td>
<td>$e = 1.77$ radii</td>
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<tr>
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<td>$\phi_r$, $\phi_P$ (from lab)</td>
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<td>32.5°, 39.0°</td>
<td>4.15</td>
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<td>$D_R = 0.25$</td>
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<tr>
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<td>2.0, 1.77</td>
<td>4.7, 4.10</td>
<td>$n_{max}$, $n_{min}$</td>
<td>$n_{max} = 0.257$, $n_{min} = 0.160$</td>
<td>$n_{max} = 0.258$, $n_{min} = 0.137$</td>
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<tr>
<td>4</td>
<td>$n_{max}$, $n_{min}$ (from 3)</td>
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<td>0.258, 0.137</td>
<td>4.2</td>
<td>$VR_{max}$, $VR_{min}$</td>
<td>$VR_{max} = 0.346$, $VR_{min} = 0.190$</td>
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<tr>
<td>5</td>
<td>$D_r$, $VR_{max}$, $Vr_{min}$ (from 2, 4)</td>
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<td>0.25, 0.348, 0.159</td>
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<td>$VR$ (target)</td>
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<td>6</td>
<td>$VR$ (target) (from 5)</td>
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<td>0.300</td>
<td>4.2</td>
<td>$n$ (target)</td>
<td>$n = 0.235$</td>
<td>$n = 0.231$</td>
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<table>
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<tr>
<th>Selected parameters:</th>
<th>Friction coefficient</th>
<th>Dyad eccentricity (radii)</th>
<th>Porosity</th>
<th>Normal Stiffness (N/m)</th>
<th>Shear Stiffness (N/m)</th>
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<tbody>
<tr>
<td>case 1</td>
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</table>

It should be noted that neither the normal stiffness nor the shear stiffness parameter appears in the final model for friction angle of peak stress or residual stress. This fact is not surprising, considering the results of the single-factor part of the study. In that section of this chapter (refer to Figure 4.4 and Figure 4.5), it was shown that increasing either stiffness parameter had little influence on either friction angle. However, since the vast majority of the data used in the development of the statistical model came from simulations using a value of 1e8 N/m for both stiffness parameters, this value is recommended for both parameters and caution should be exercised in using any other stiffness parameters. Based on that stipulation, the full set of simulation parameters...
in question has now been defined in Table 4.3 for both arbitrary cases of friction coefficient in Step 1 as described. Direct shear test simulations were conducted for both cases to test the calibration. To assess how close the resulting friction angles should be to the target values, a 95%-confidence prediction interval was computed by the statistical analysis software. Such an interval means that based on the variation in the data used to develop the statistical model, there is a 95% chance that a new data point will fall within the interval. The greater the variation in the original data, the greater the prediction interval will be, i.e. the predicted value is less certain. The stress-displacement curves for physical MGR sand and for the calibrated simulations are displayed in Figure 4.15 and the average friction angles of each simulation case are compared graphically to the expected values in Figure 4.16.
Figure 4.15: Stress-displacement curves for Physical DST of MGR sand (left), Calibrated parameter case 1 (middle), and Calibrated parameter case 2 (right).

Figure 4.16: Friction angles produced by simulations calibrated by the statistical model, with 95% confidence limits for the predicted values. See Appendix B for specific values.
From both Figure 4.15 and Figure 4.16 it is apparent that both Cases 1 and 2 selected reasonable parameter sets. All values for friction angle that were obtained (summarized in Figure 4.16) were within the 95% confidence interval except one value from Case 2. Further, the means of the friction angle values obtained were well within the predicted limits and were reasonably close to the respective target values. However, Case 1 was notably more accurate than was Case 2. The reason for this is not certain; one explanation may be random error. Also, from the curves of Case 2, visible in Figure 4.15, it is observed that as the confining pressure increases, the curves look increasingly different from the physical sand curves in terms of their overall shape. Differences perceptible to the eye include excessive jaggedness and discrepancies in peak and residual stress values. The observed apparent relationship to confining pressure suggests that there is more to learn about its interaction with eccentricity and friction coefficient. Regardless, the statistical-model method of selecting parameters has been demonstrated to be profitable for the task of calibration of dry sands to the direct shear test. Even if the method were used to select several trial cases that would then be tested by DST to select the best among them, these several cases would require far fewer DST simulations than would the traditional trial-and-error approach, and correspondingly less computational expense would be invested into the calibration phase of the project.

4.2.4. Effect of Lowering Contact Stiffness for Computational Benefit

Earlier in this chapter it was noted that the statistical model makes no prescription regarding the contact stiffness parameters, and that it is conservative to remain at the stiffness level of 1e8 N/m used predominantly for both parameters in the calibration
study. But if it were possible to use lower values for stiffness, doing so would be advantageous with respect to computational effort since the maximum allowable time increment would be increased. In order to examine this possibility, several DST simulations were conducted using the parameter sets prescribed in Cases 1 and 2 above, except that both the normal and shear stiffness were reduced by a factor of ten to 1e7 N/m to increase the time increment by a factor of roughly \( \sqrt{10} \) or 3.16 (subject to deviations in the specimen). The resulting stress-displacement curves are in Figure 4.17 and the friction angle values are summarized in Figure 4.18.

Figure 4.17: Stress-displacement curves for Physical DST of MGR sand (left), Modified parameter case 1 (middle), and Modified parameter case 2 (right).
By visual inspection of Figure 4.15 it is apparent that the typical trend among stress-displacement curves for dense sand, in which the shear stress reaches an early peak and then reaches a lower steady-state level, is present in the behavior of the physical sand. This trend is also visible in the behavior of the calibrated simulations for both parameter cases (Figure 4.15). The trend is absent, or at least not obvious, in the curves for the modified cases (Figure 4.17). However, among the curves in the modified cases it was observed that as the confining stress increased, the trends became more and more like the behavior of loose sand, lacking a clear peak. For the highest confining stresses among the simulation results in Figure 4.17, the difference between the peak stress value and the residual stress value clearly results from the extensive fluctuations in the curve rather than from any trend, and the friction angle for peak stress was rather low compared to the target. The lowest confining stress, on the other hand, offered a hint of the trend typical of dense sand and produced peak stresses notably closer to the target. For this
reason simulation data were added for a lower confining stress of 30 kPa, anticipating that the expected trend for dense sand would again become obvious. The resulting stress-displacement curves for each modified parameter case at 30 kPa are shown in Figure 4.19 (along with the 75-kPa curves previously shown in Figure 4.17). A summary of results from each 30-kPa simulation case is given in Figure 4.20.

Figure 4.19: Stress-displacement curves of Modified Case 1 (left) and Modified Case 2 (right) parameters at normal stresses of 75 kPa (higher curves, repeated from Figure 4.17) and 30 kPa.
Figure 4.20: Friction angles produced by simulations using Modified Cases 1 and 2 at confining pressure of 30 kPa, with 95% confidence limits for the predicted values. See Appendix B for specific values.

The results in Figure 4.19 indicate that indeed the typical “dense-sand” stress-displacement trend is still realized at low normal stresses even though reduction of the contact stiffness parameters eliminated this behavior at higher normal stresses. Further, the friction angles produced for both peak and residual stress (Figure 4.20) are close to the friction angles of the physical soil. These observations support the idea that lowering the stiffness parameters for the sake of reducing computational burden is acceptable if 1) shear strength (peak and/or residual) is the primary quantity of interest and 2) the normal stresses are adequately low. The latter should be tested in a similar manner as above on a case-by-case basis.
5. RIGID WHEEL ON SAND

The task of demonstrating an application of the statistical model discussed in Chapter 4 required a system that would afford the ability to compare physical test data to results of a simulation that was based on the statistical model. A wheel/soil system was employed because of the availability of a testing and data acquisition apparatus and because wheel/soil interaction was the original motivation of this project.

5.1. Physical Experimentation Using WEST-MGRS

5.1.1. Description of the System

The Wheel Endurance and Sand Traction Merry-Go-Round System (WEST-MGRS or simply MGR) developed by the CEDAR lab in Clemson University’s Mechanical Engineering department was used to collect data on the tractive performance of several rigid wheels with 2-D tread designs (i.e. grousers). See Figure 5. for a photograph of the MGR system. The MGR consists of a wheel mounted at a fixed horizontal position, and rolling along the soil surface in a rotating trough full of sand (i.e. turntable). The shaft of an electric motor whose speed is controlled by the user is connected to a reducing gear box; the output shaft of the gear box drives the wheel’s rotation. The turntable consists of a trough containing a rectangular soil cross-section 56 cm wide and 14 cm deep on average. This cross section is geometrically rotated about a vertical axis 3 m away, resulting in a curved trough that forms a circle nearly 20 m in circumference. The entire circular trough is suspended by cables connected to bearings on a pole at the axis of rotation, such that the trough is able to spin about its geometric
center. The result is a circular path for the wheel to traverse continuously as the trough rotates.

![MGR testing apparatus operating with a typical pneumatic tire.](image)

Figure 5.1: MGR testing apparatus operating with a typical pneumatic tire.

The turntable and the sand it contains together have a mass over 2800 kg. Although it is free to spin on the bearings that support it, there is a great deal of inertia. Since the wheel drives the rotation of the turntable, the turntable’s inertia is the basis of testing wheel performance: the time required for the turntable to reach a certain speed decreases as wheel tractive performance increases. The MGR is equipped with a data acquisition system that monitors and records the rotation speeds of the wheel and the turntable, as well as numerous other quantities not used in this research.
5.1.2. Measurement of Rotational Inertia

Since the rotational inertia of the turntable was instrumental in measuring the tractive performance of the wheel, a reasonable estimate needed to be made of it. Therefore, dual methods were used for mutual verification. The quantity was computed geometrically using the dimensions of the turntable, material densities, etc. This method’s main source of error was due to the sand in the turntable: the sand itself accounts for the vast majority of the system mass, but obtaining an accurate value of the sand’s bulk density is difficult. Thus a wide range of values may be obtained, depending on the estimate used for the bulk density of sand. The best rotational inertia value computed in this way was $2.94 \times 10^6$ slug*in$^2$.

Secondly, an experimental measurement of the turntable’s rotational inertia was obtained. This was done using data acquired by the MGR data system during a free-rotation experiment of the turntable. The turntable was given an initial rotation by manual input, then was allowed to coast freely until it came to rest. The angular velocity was recorded during the entire free rotation, and was plotted against time in Figure 5.2. The plot is remarkably linear, with some visible periodic variations that presumably correspond to angular position of the turntable (on the basis of the apparent decreasing frequency). A linear regression was generated on the data, with its slope having units of rad/s$^2$. The fact that the slope of the actual data (i.e. the angular acceleration of the turntable) is predominantly consistent with the linear regression implies that the sum of the retarding moments applied to the turntable is likewise essentially constant. Therefore,
The rotational form of Newton’s second law can be straightforwardly used to compute the moment of inertia about the axis of rotation if the moments are known:

$$\Sigma M_O = I_O \alpha$$  \hspace{1cm} (5.1)

The only moments potentially acting about the turntable’s axis during this experiment were the couple due to bearing friction and moments due to viscous drag forces from the air. The latter were assumed to be negligible due to 1) the slow speed of motion and 2) the constant acceleration observed. Therefore, an experiment was designed to measure the couple due to bearing friction.

The bearing friction couple was measured by wrapping a flexible cord around the perimeter of the turntable, routing it over a pair of pulleys, and suspending a bag of weights from it. Since the cord came off the turntable in a direction tangent to the turntable, the total weight of the bag produced a known moment about the axis of rotation, assuming that the pulleys had negligible friction and that the cord had negligible weight. Weight was continually added to the bag until the turntable would no longer return to rest once bumped. This condition was taken to correspond to the bearing couple during rotation (as opposed to the maximum bearing couple when static). The value of the couple was computed by multiplying the weight of the bag by the radius of the turntable where the cord was attached. This measurement was repeated at six evenly distributed angular positions of the turntable, and the results averaged to account for variation in the couple with changing angular position. The average (68.2 in*lb) was taken as the couple moment $M_O$ in Equation (5.1) above. Using this value, the moment of inertia of the turntable about its axis of rotation was estimated to be $2.98 \times 10^6$ slug*in$^2$. 
This was quite close to the estimate obtained by geometric computation (1.4% higher) and was considered to be the more reliable of the two numbers. Therefore this estimate of inertia was used in subsequent calculations.

Figure 5.2: Angular velocity of turntable vs. time during free-rotation test for finding the moment of inertia.

5.1.3. Experiments and Results: Grouser Performance

Bekker claims that grousers do not directly improve traction as is often assumed because they tend to simply become filled with soil. Rather, he says, the reason a grousered wheel gets better traction is that the grousers effectively increase the diameter of the wheel by a value of $2h$, where $h$ is the height of one of the grousers [3]. However, it is not clear whether Bekker intended this statement to apply to certain types of soil only.
or to all types. The current work intends to consider Bekker’s conclusion about grousers as it applies to their behavior in sandy soils. The specific wheel designs used on the MGR for this work offer a comparison of the performance of two different shapes of grouser, as well as a comparison of the performance of grousers at different levels of spacing. These cases are presented along with the performance of the wheel with a simple round shape at two different diameters: the diameter corresponding to the tip of the grouser and the diameter corresponding to the base of the grouser. According to Bekker, the smaller-diameter wheel should perform worse than all the others, but all the others should compare closely to one another. A pictorial representation of the six cases tested can be found in Figure 5.3.
Figure 5.3: Wheel profiles for the shapes tested using the MGR. a) Wheel with 64 blunt grousers (spaced at 5.625° of wheel arc), b) 64 sharp grousers (spaced at 5.625°), c) 32 sharp grousers (spaced at 11.25°), d) 16 sharp grousers (spaced at 22.5°), e) no grousers: larger diameter, and f) no grousers: smaller diameter.

All six cases of grouser configuration were tested using a single wheel; the grousers were designed so as to be removable. See Figure 5.4 for a photograph of one of the wheels operating on the MGR. The wheel was composed of an aluminum hub that bolted to the MGR drive assembly. Two sheet metal disks (stainless steel) connected the hub to an outer ring of cast epoxy. The removable grouser panels made of ultra-high molecular weight polyethylene (UHMW-PE) then were fastened to the outer ring using machine screws. All these parts of the wheel are visible in Figure 5.4. The diameter of the wheel at the base of the grousers was 52.1 cm. Each grouser was either a rectangle
with a base of 1.25 cm (tangent to the wheel) and a height of 2.05 cm (radial direction) or an isosceles triangle of the same base and height. The grousers were spaced evenly around the circumference of the wheel as shown in Figure 5.3. The width of the wheel (parallel to the wheel axis) was 15.6 cm.

![Figure 5.4: Wheel with 32 sharp grousers (see Figure 5.3c) during an acceleration test.](image)

Two experiments were performed with each wheel type, one in which the system accelerated and one in which the system decelerated. Each test began with the wheel operating on groomed sand, meaning that the tracks from previous rotations of the turntable had been disturbed by manual raking, so as to restore the sand to an approximately un-traversed condition. The acceleration test was designed to compare the
net tractive effort developed by the different wheel types. Starting the system from rest, the angular velocity of the wheel was ramped up linearly (i.e. constant angular acceleration) until it reached the desired angular velocity, selected to correspond to a travel velocity of 1 km/h for a wheel of the same outer diameter rolling on a hard surface without slip. Since the wheel was resting on the soil surface of the turntable and was supporting the weight of the wheel and the mounting frame (625-685 N, depending on wheel type), the wheel’s rotation caused the turntable to begin rotating as well. Once the wheel reached the desired angular velocity, that angular velocity was maintained until the turntable had completed two full rotations; then the test was terminated. The acceleration experiment was repeated five times for each wheel type. A typical data set for five acceleration tests is shown in Figure 5.5. The equivalent wheel speed increases in a nearly linear fashion since it is driven by the motor, reaching its intended operating velocity in about 4 seconds. The wheel speed profile was the same for every wheel. The MGR surface, because of its large mass, accelerates more slowly than the wheel does—so much more slowly, in fact, that the plot gives the appearance that the MGR does not move at all for about 3 seconds after the wheel begins to rotate. During this period of excessive slip, in reality the MGR does move slightly, but it is believed that the speed of the MGR is too slow to be picked up by the instrumentation. The time required for the MGR to reach its steady-state speed is an indication of the traction produced by the wheel: a wheel with better traction will bring the MGR up to speed in a shorter time.
The second experiment was designed to compare rolling resistance due to soil deformation among the wheel designs. This experiment began with the system operating at constant speed and with the sand being groomed. At the start of the test, the grooming was stopped and the wheel drive motor was turned off. The drivetrain of the wheel included a ratcheting device that would allow the wheel to rotate with relative freedom if driven by kinetic energy from the turntable, even when the drive motor shaft stopped rotating. The rolling resistance test provided a comparison of how quickly the turntable came to rest once the motor stopped driving the system. In no case did the turntable complete a full revolution before coming to rest; therefore, the wheel was always
operating on groomed sand during the rolling resistance tests. This test was also repeated five times for each wheel type. A typical data set for five rolling resistance tests is shown in Figure 5.6.

![Figure 5.6: Rolling resistance test (five repetitions) for wheel with 64 sharp grousers. MGR speed and equivalent wheel speed are assumed equal since the wheel is free-spinning.](image)

For wheels operating on sandy soil, the friction between wheel and soil has a limited ability to influence traction. If the coefficient of friction is low, excessive slip may occur between the wheel surface and the soil. As the coefficient increases, a point will be reached at which slip will cease between the wheel surface and the soil. This does not mean however that no more slip occurs at all; rather, all slip that does occur will be at
a location in the soil that is not in contact with the wheel surface, i.e. the slip will occur between neighboring grains of sand. Once the friction coefficient between the wheel and the soil is high enough to result exclusively in this condition of sand-on-sand slip, further increases in friction coefficient will not improve tractive performance. In order to combat the apparently low coefficient of friction between the UHMW-PE grousers and the sand, a condition of sand-on-sand slip was guaranteed by using double-sided duct tape to coat all wheel surfaces involved in generating traction. As a demonstration that this approach produced reasonable results, the large grouser-free wheel was also tested using two alternative materials: 1) a neoprene rubber layer and 2) a sandpaper layer with grain sizes comparable to those observed in the sand itself. Both performed comparably to the double-sided duct tape in the acceleration test, supporting the idea that the double-sided duct tape was a reasonable approximation to a material having high enough friction coefficient to result in sand-on-sand slip. This result will again be important later in the simulation section of this chapter, where an unusually high friction coefficient will be used between the simulated wheel and soil to achieve sand-on-sand slip. The results of all the tests performed on the MGR, including acceleration tests and rolling resistance tests with double-sided duct tape, as well as the tests using alternate materials, are summarized in Table 5.1. It should be noted, when comparing the table to Figure 5.6, that the deceleration in the figure was from an initial speed of about 3km/hr, while the deceleration recorded in the table was from an initial speed of about 0.9 km/hr due to the extremely long computational time that would have been needed to simulate coming to rest from the higher initial speed. The time values in Table 5.1 were recorded from 0.9
km/hr in order to facilitate comparison between it and Table 5.3, which appears later in this chapter and provides values from simulations of the MGR experiments.

Table 5.1: Average performance of different grouser configurations. All configurations had tractive surfaces covered with two-sided duct tape unless otherwise indicated.

<table>
<thead>
<tr>
<th>Grouser Setup</th>
<th>Acceleration Time (s), 0 to 0.9 km/hr</th>
<th>Deceleration Time (s), 0.9 to 0 km/hr</th>
</tr>
</thead>
<tbody>
<tr>
<td>blunt, 64 grousers</td>
<td>15.0</td>
<td>4.0</td>
</tr>
<tr>
<td>sharp, 64 grousers</td>
<td>11.9</td>
<td>4.6</td>
</tr>
<tr>
<td>sharp, 32 grousers</td>
<td>11.2</td>
<td>5.6</td>
</tr>
<tr>
<td>sharp, 16 grousers</td>
<td>12.3</td>
<td>4.3</td>
</tr>
<tr>
<td>none, major diameter</td>
<td>17.8</td>
<td>3.6</td>
</tr>
<tr>
<td>none, minor diameter*</td>
<td>23.9*</td>
<td>3.5*</td>
</tr>
<tr>
<td>major diameter with rubber</td>
<td>18.7</td>
<td>4.2</td>
</tr>
<tr>
<td>major diameter with sandpaper</td>
<td>17.2</td>
<td>3.7</td>
</tr>
</tbody>
</table>

*Data for this wheel case not consistent, likely due to different person responsible for sand grooming

Comparing the acceleration times listed in Table 5.1, it is apparent that any grousers offer better traction than no grousers. Among grouser types, sharp ones perform somewhat better than blunt ones. Although the spacing of the sharp grousers appears to have an optimum, the differences in performance between the levels of spacing appear to be small. The major diameter round wheel produced the same acceleration regardless of whether it was covered with duct tape, rubber, or sandpaper. As mentioned, this fact will be important for the simulation of the MGR system. Finally, the minor diameter round wheel performed far worse than any of the other wheels. Although the wheel was expected to perform worse, it seems questionable whether the degree of difference observed could have been due to an outside factor. Further data would be helpful to answer this question. Comparison of the deceleration times is less conclusive because all the times fall within a 2-second range. However, it is noteworthy that all the wheels with
grousers took longer to stop than any of the wheels without grousers. This fact implies that the grousered wheels actually have a lower rolling resistance in sand than the non-grousered wheels, an observation that seems counterintuitive.

5.2. DEM Simulation of MGR Experiments

5.2.1. Description of the Simulated System

A DEM simulation was constructed in PFC2D to reproduce the physical experiments conducted on the MGR as closely as possible. Each simulation was run twice: once with 25 thousand ("25k") total soil particles and once with 50 thousand ("50k"). Computation of the 25k-particle simulations required on the order of 4-6 days; the 50k-particle simulations required 35-42 days. For the purposes of the 2-D simulation, the horizontal direction corresponded to distance along the trough (i.e. the curved path of the trough was taken as planar). Thus defined, the horizontal length of the sand box was 5 meters for the first simulation set, with 25k particles. For the second set, with 50k, information from the first set about the wheel’s travel distance revealed that the sand box needed to be only 3 meters. The target sand depth, taken directly from the physical system, was 14 cm, although the specimen-preparation process resulted in small non-uniformities in depth along the length of the box. The width of the trough’s cross-section was not present in the simulation since it corresponds to the third spatial dimension. The “thickness” parameter (refer to Section 3.1.3.) provided to the simulation for computation of particle masses was 15.6 cm, equal to the thickness of the wheel. This value was selected because in the physical system, only the soil grains located between the bounding planes of the wheel (planes perpendicular to wheel axis) have the potential to
be accelerated directly by the wheel, if 3-D effects are neglected. The previous statement is not intended to include acceleration of the sand particles due to their moving along with the MGR trough; such acceleration is accounted for in the simulation by horizontal motion of the wheel.

The soil parameters used in the MGR simulation were those obtained in Chapter 4 through the statistical model calibration process (Case 1). Since the MGR simulation involved a comparatively large amount of time and far more particles than did the direct shear test simulations (25k or 50k compared to 10k), computational advantages were sought. It was decided that since shear strength (peak and residual) was the main outcome of interest with respect to the soil, and that since the estimated average normal stress beneath the wheel was only about 32 kPa, the reduction of contact stiffness to 1E7 was acceptable according to the findings presented in Chapter 4. Table 5.2 provides a list of the soil parameters used in the simulation, as well of other parameters of interest.
Table 5.2: Parameters used in the MGR simulations

<table>
<thead>
<tr>
<th>Soil Parameters</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Friction Coefficient</td>
<td>0.7</td>
<td>[-]</td>
</tr>
<tr>
<td>Dyad Eccentricity</td>
<td>2.02</td>
<td>[radii]</td>
</tr>
<tr>
<td>Porosity with no Load</td>
<td>0.235</td>
<td>[-]</td>
</tr>
<tr>
<td>Normal Contact Stiffness</td>
<td>1.0E+07</td>
<td>N/m</td>
</tr>
<tr>
<td>Shear Contact Stiffness</td>
<td>1.0E+07</td>
<td>N/m</td>
</tr>
<tr>
<td>Damping Coefficient (default PFC2D value)</td>
<td>0.7</td>
<td>[-]</td>
</tr>
<tr>
<td>Minimum Particle Diameter (25k/50k)</td>
<td>1.92/1.05</td>
<td>mm</td>
</tr>
<tr>
<td>Maximum Particle Diameter (25k/50k)</td>
<td>7.69/4.21</td>
<td>mm</td>
</tr>
<tr>
<td>Particle Size Distribution Type</td>
<td>Uniform</td>
<td>[-]</td>
</tr>
<tr>
<td>Upscale factor (25k/50k particles)</td>
<td>17.8/9.7</td>
<td>[-]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Wheel Parameters</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Friction Coefficient</td>
<td>1</td>
<td>[-]</td>
</tr>
<tr>
<td>Normal Contact Stiffness</td>
<td>1.0E+07</td>
<td>N/m</td>
</tr>
<tr>
<td>Shear Contact Stiffness</td>
<td>1.0E+07</td>
<td>N/m</td>
</tr>
</tbody>
</table>

The same grouser configurations were used in the simulation as were used in the physical experiment, shown previously in Figure 5.3. These shapes were created in the simulation from a group of connected walls that moved together as one rigid body. A single frame from an animation of the simulated system is shown in Figure 5.7. In the figure, the wheel is rotating clockwise at a constant angular acceleration. Translation is not prescribed, but results from forces imparted by the soil. Soil particles are colored with a regular pattern based on their original position; this facilitates visual observation of soil motion during the simulation. The PFC software contains built-in logic to specify only the velocity of walls, but it does allow the user to read the force and couple reactions acting on the walls from the soil particles. For the MGR simulation, the reactions on the walls comprising the rigid wheel were monitored throughout the simulation and this information was used by a set of custom functions to continuously specify the velocities.
of the wheel (x-, y-, and angular), based on the principles of rigid-body dynamics (i.e. Newton’s second law). Specifically, using the reactions from the soil and using mass properties defined from the physical system as described below, the accelerations (horizontal, vertical, and angular) were computed at every time increment. The accelerations were then integrated explicitly (just as the motion of the particles is) to determine the velocities, which were then assigned to the wheel walls. Therefore, those walls moved as a unit with the motion of a rigid body having the set of mass properties described in the following paragraphs.

Figure 5.7: DEM animations of rigid wheel with 16 sharp grousers: Initial position (top), Final position (middle), Detail of grousers in soil during acceleration (bottom).
The nature of the MGR system provides a unique set of operating conditions for any wheel that is tested on the system. Ordinarily a wheel or set of wheels is affixed to a mobile frame (i.e. a vehicle), and relative motion between the wheel and the soil occurs as the vehicle travels. In such cases, the vehicle mass that loads the wheel vertically, providing a contact force between wheel and soil, is the same mass that the tractive effort must accelerate from rest in order for the vehicle to travel. Therefore, the vehicle mass governs vertical motion and horizontal motion. In the MGR system however, the vertical motion of the wheel is governed by the mass of the wheel and its mounting frame, while the relative horizontal motion is governed by the inertia of the turntable. The rotation of the wheel was governed by its moment of inertia about the center point. In the simulation, it was important to keep the sand bed stationary because of computational metrics for soil condition (as described in Chapter 4), so the wheel was allowed to travel horizontally. The following equations of motion were applied to the wheel in the simulation, in which $\sum F_i$ is the sum of forces acting on the wheel in the $i$-direction, $m_w$ is the mass of the wheel, $a_i$ is the $i$-component of the acceleration of the wheel’s center of gravity, $m_{mgr}$ is the equivalent mass of the turntable, $\sum M_z$ is the sum of moments acting about the wheel axis, $I_G$ is the moment of inertia of the wheel about its axis of rotation, and $\alpha$ is the angular acceleration of the wheel:

\begin{align}
\sum F_y &= m_w a_y \\
\sum F_x &= m_{Mgr} a_x \\
\sum M_z &= I_G \alpha
\end{align}
The mass of the wheel (and the part of its frame that moved vertically) in Equation (5.2) was obtained simply by placing a scale under the mounted wheel to measure the weight resting on the sand surface. The mass responsible for this weight was used in the simulations. The values for wheel mass ranged from 63.6 to 70.0 kg, depending on the grouser configuration. Similarly, the wheel’s moment of inertia about the wheel center, Equation (5.4), was computed directly from the wheel geometry and material properties. The moment of inertia ranged from 0.561 to 0.967 Kg-m$^2$, depending on the grouser configuration. However, the equivalent mass of the turntable for use in Equation (5.3) was computed from the known rotational inertia of the turntable (found earlier in the chapter). To determine this value, an “equivalent radius of gyration” was used. The radius of gyration for an object is the theoretical radius of an imaginary thin ring having the same mass and moment of inertia as the original object. The radius of gyration for an object is related to its mass and moment of inertia by Equation (5.5), where $I_o$ is the moment of inertia of the object about the axis in question, $m$ is the mass of the object, and $k_o$ is the radius of gyration with respect to the same axis.

$$I_o = mk_o^2$$  \hspace{1cm} (5.5)

Typically, the mass of an object is known and the moment of inertia is known; these may then be used to compute the radius of gyration. However, to find the equivalent mass needed to describe the horizontal motion of the wheel using Equation (5.3), the situation was different. In the application of Equation (5.6), it was as if the imaginary thin ring had a known radius (equal to the distance from the turntable axis to the wheel centerline,
and the exact mass was sought \( (m_{MGR}) \) which would result in identical moment of inertia to that of the turntable \( (I_o) \).

\[
I_o = m_{MGR} (r_{MGR})^2
\]  

Equation (5.6)

Knowing the moment of inertia of the turntable to be \( 2.98 \times 10^6 \) slug*in\(^2\) from experiment and using the measured turntable radius of 126.25 inches, the equivalent mass for use in Equation (5.3) was computed to be 186.9 slugs (2728 kg).

5.2.2. Experiments and Results: Grouser Performance

A simulation was created for each of the same six wheel configurations shown in Figure 5.3 for the physical MGR system. No alternative cases were simulated corresponding to various materials as was described for the physical system; all six wheel shapes were simulated using a high coefficient of friction on all wheel surfaces to achieve a predominant slip mechanism of sand-on-sand. For the sake of simplicity, the two separate experiments performed on the MGR were combined into a single experiment in the simulation, consisting of three phases: 1) constant acceleration to desired wheel angular velocity (0 to 1 km/hr equivalent speed on a rigid surface without slip), 2) a brief operation at constant wheel angular velocity during which the horizontal motion was expected to reach a steady-state condition, followed by 3) free deceleration back to rest, under the effects rolling resistance. During the acceleration and constant-speed phases of the simulation, Equations (5.2) and (5.3) governed the translation of the wheel, but the rotation of the wheel was defined kinematically according to the desired velocity profile (as it was in the physical experiment, using a motor controller). Thus Equation (5.4) was not used during these phases. However, for the deceleration phase, all three governing
equations were in effect. Recall that in the physical experiment’s deceleration phase the wheel was no longer driven by the motor but was free to rotate as pushed by the sand. Each grouser configuration was run once with 25k particles, then subsequently once with 50k. Although multiple repetitions of each would have been desirable, computational expense was prohibitive. See Figure 5.8 and Figure 5.9 for typical plots produced by the simulations. The simulation results for all six wheel configurations are summarized in Table 5.3.

Figure 5.8: Acceleration and rolling resistance data for 25k-particle simulation of wheel with 16 sharp grousers.

Figure 5.9: Acceleration and rolling resistance data for 50k-particle simulation of wheel with 16 sharp grousers.
Table 5.3: Average performance of different grouser configurations in simulation.

<table>
<thead>
<tr>
<th>Grouser Setup:</th>
<th>Acceleration Time (s), 0 to 0.9 km/hr</th>
<th>Deceleration Time (s), 0.9 to 0 km/hr</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Number of Particles):</td>
<td>25k</td>
<td>50k</td>
</tr>
<tr>
<td>blunt, 64 grousers</td>
<td>4.1</td>
<td>4.2</td>
</tr>
<tr>
<td>sharp, 64 grousers</td>
<td>3.5</td>
<td>3.5</td>
</tr>
<tr>
<td>sharp, 32 grousers</td>
<td>3.4</td>
<td>3.3</td>
</tr>
<tr>
<td>sharp, 16 grousers</td>
<td>3.6</td>
<td>3.4</td>
</tr>
<tr>
<td>none, minor diameter</td>
<td>4.2</td>
<td>4</td>
</tr>
<tr>
<td>none, major diameter</td>
<td>3.9</td>
<td>3.8</td>
</tr>
</tbody>
</table>

A comparison of the results in Table 5.1 and Table 5.3 offers an indication of the usefulness of the simulation for predicting the tractive performance of grouser configurations. As anticipated, the value of acceleration achieved by the wheel is not accurately predicted, since it has been shown that the behavior of a wheel operating on deformable soil is strongly subject to three-dimensional effects [1]. The acceleration time was under-predicted (i.e. unrealistically high accelerations predicted). However, as seen in Figure 5.10, the relative performance between grouser configurations is predicted with a reasonable level of accuracy. Therefore the simulation can be used to compare the performance of one grouser design to another, and reasonable recommendations for design preferences can be made from the simulation results. Also noteworthy is the fact that the 25k-particle simulations produced nearly the identical predictions as the 50k simulations; therefore in this case it was more cost effective to use the lower number of particles. Further investigation is needed to find a way to predict how many particles are enough.
Figure 5.10: Comparison of acceleration time for physical and simulated MGR experiments. Note that data for physical Case 6 may have explainable inaccuracy due to a different person grooming sand. See Figure 5.3 (a-f) for configurations 1-6, respectively.

Better accuracy was obtained for deceleration due to rolling resistance; the stopping times predicted by the simulation were reasonably close to the experimental values (time somewhat over-predicted; deceleration under-predicted, Figure 5.11). In fact, after completion of the simulations it was recognized that the friction of the wheel bearings (about 6.7 N-m) was not accounted for in the simulation. The friction did not
need to be accounted for during the phases of the simulation involving prescribed wheel rotation speed, only during the freely-coasting phase. An impulse-momentum analysis was used to estimate the resulting deceleration time if the bearing friction had been accounted for. The analysis indicated that for each wheel case the deceleration time would have been around 85% of the time computed without inclusion of bearing friction, which would have brought all the simulated deceleration times within the range of observed deceleration times in the physical system.

Unlike in the acceleration test, the relative differences in deceleration between the various grouser configurations were not accurately predicted by the simulation. This discrepancy might be explained by the fact that only one trial for 25k-particles and one trial for 50k of each grouser type were computed. Simulating additional trials would be beneficial, especially since there was some variation in deceleration between trials of any given wheel in the physical experiment; however, the variation is not great enough to strongly support this idea as an explanation. Additionally, the trend observed in the stopping times for the different grouser configurations does not have an obvious, intuitive explanation. For example, there is not an obvious, intuitive reason why configuration 3 (32 sharp grousers) would have significantly lower rolling resistance than Configuration 2 or 4 (64 or 16 sharp, respectively). For this reason it may be called into question whether the physical results for deceleration reflect an unknown outside influence (lab temperature, sand preparation, etc.). Regardless, without further data, the simulation should not be used to compare or recommend grouser designs with respect to rolling resistance.
The most puzzling aspect of the results presented in Figure 5.10 and Figure 5.11 is the fact that the simulation predicted the acceleration of the system so poorly while predicting the deceleration reasonably well. No indisputable reason for this discrepancy has been determined; however, there is a notable difference between the conditions applied to the soil under a wheel being driven by a torque versus a freely-rolling wheel. Under a torque-driven wheel, there is unquestionably an application of shear stress in the
direction tangent to the wheel; this fact is obvious because if the torque applied is large, the wheel slips excessively. For a physical, 3-D wheel, when a normal stress is applied in the vertical direction, that vertical stress is not matched from the front, back, or sides: the sand moves instead of developing the expected normal stress. Since the soil’s shear strength is proportional to the normal stress, the shear strength remains quite low. The use of grousers has been shown in this chapter to improve the traction of a wheel in sand; this improvement may be due to the grousers’ trapping of the sand to prevent its motion toward the front of the wheel and thus allowing a higher normal stress to develop in that region. Since the soil is less free to move forward out from under the wheel, the entrapping action of the grousers is likely to result in reduced sinkage for conditions where the wheel slip is small and reduced bulldozing regardless of the degree of slip. The data in Figure 5.10 suggest that an optimal grouser spacing exists at some value about the value present on the wheel with 32 grousers. This observation is consistent with the concept of entrapment: grousers spaced too widely allow sand to escape entrapment, but grousers spaced too close together do not allow adequate sand into the region that is subject to entrapment. Finally the entrapment theory also suggests that a great improvement in wheel traction would be expected if the wheel were operated within a track whose width were only slightly larger than the width of the wheel itself, such that the track walls eliminated sideward motion of the soil. This system would result in a plane-strain situation for the soil, allowing greater normal stresses to develop. In fact, it is to such a plane-strain situation that the 2-D DEM model has been calibrated in this dissertation using the direct shear test, and it is expected that such an experiment would
agree far better with the simulated wheel acceleration values shown above. Applying a similar train of thought to the case of a wheel operating in open soil, the addition of a washer-shaped ring of sheet metal or other stiff material on either side of the grousers might aid in the development of normal stress since it would restrain the sand from moving toward either side. However, the important point is that shear strength is necessary for traction and that the simple cylindrical wheel in open soil has limited ability to bind the soil so that it has strength.

On the other hand, a free-rolling wheel engages the soil in a different way. The free wheel tends to press downward on the soil without the additional demand for the sand to resist shear. As the sand grains slip over each other, energy is dissipated through friction. The energy dissipated is expected to correlate strongly to the volume of soil displaced; therefore a weaker soil would offer more rolling resistance since it gives way more readily. Since the MGR simulation demonstrated a stronger soil in the acceleration test (high acceleration) as compared to the physical system, it was expected that the simulation would also demonstrate a much lower rolling resistance. The simulation certainly predicted far less sinkage than the physical system displayed. However, as discussed previously the wheel decelerated at comparable rates between the simulation and the physical system. A likely explanation for why the simulation did not under-predict the rolling resistance is that the DEM model actually has two mechanisms for dissipation of mechanical energy: friction and contact damping. The former is believed to be the dominant mechanism in the physical system; the latter is believed to be nearly non-existent in the physical system due to the high stiffness of sand grains. The
software’s default damping value was left intact during all the simulation; the default value was chosen to be the optimal value for bringing particle systems to static equilibrium quickly. Perhaps if the contact damping had been set to a lower value then the rolling resistance would have been lower, as expected based on the high acceleration performance of the simulated system. Further investigation of the effects of contact damping is strongly suggested as an item for future work.
6. FEM STUDY: METHOD TO SELECT SOIL DOMAIN DIMENSIONS

6.1. Challenges

The performance of deformable wheels on deformable soils has been an interesting topic of study for a number of years. Attempts were made to predict wheel performance by analytical or empirical methods as early as the 1950’s [20] [3]. More recently the problem has been approached by computational methods with some success [8] [11]. The computational approach is often limited to two-dimensional models, which have been shown to be insufficient [14]; yet three-dimensional models quickly grow to unfeasible sizes from the standpoint of computational resources. To help alleviate the computational burden, Orr et. al. proposed a method to select soil domain dimensions for a dynamic wheel-soil model, seeking to dimensions of the soil domain for such a simulation in a way that avoids modeling unnecessary soil volume [2]. In that study by Orr, a single system was used to demonstrate the method’s ability to produce a soil size that captures all significant soil movement in a lunar environment without modeling an excessive amount of unneeded material. Now the current work addresses some questions about the method’s applicability to other systems:

- What adjustments must be made to the method for terrestrial applications?
- What influence do wheel dimensions have on the method’s effectiveness?
- What is the influence of wheel load on the method’s effectiveness?
- How does soil type change the method’s effectiveness?
6.2. Overview of the Soil domain sizing Method

The soil domain sizing method as proposed by Orr consists of three main steps, outlined in Figure 6. In the figure, each time that a step requires the user to make a selection, a suggested value is listed in parentheses [2].

1. Initiation
   - Select initial dimensions (3 times wheel radius r in each direction from wheel starting and predicted stopping points)
   - Select characteristic length (L = r) and accuracy limit (e = 0.1 mm)
   - Run Simulation

   Is the displacement at one characteristic length away from any edge greater than e?

2. Expansion
   - Increase each dimension with significant displacement by L (maintain mesh size)
   - Run simulation

3. Reduction
   - Set each dimension to the smallest length that captures all displacement greater than e
   - Run simulation
   - This is the final size that can be used for mesh refinement and further simulations

Figure 6.1: Method for Sizing a Soil Bed
The goal of the soil domain sizing method is to produce the smallest size that accurately reflects the behavior of a semi-infinite domain. If successful, the dimensions recommended by the method should then be still large enough that a change in the kinematic boundary conditions has little effect on the system’s behavior. This criterion is used to evaluate the effectiveness of the method: once the method has been performed for the system in question, the final size is repeated with the boundary conditions changed from pinned at boundary nodes to rollers (i.e. translation prevented in one direction instead of three). If the results of interest are obtained within a reasonable percentage (5% in this work), then the method is considered to be successful; otherwise, an explanation is sought and a way to correct the discrepancy is proposed.

6.3. Simulation Details

Several parts of this section are reproduced from [2] regarding computation, kinematics, loading, and the soil model. They are included here for completeness. The simulation details apply to all simulations presented throughout this study unless otherwise noted.

6.3.1. Computation

The models were developed in ABAQUS/CAE and executed using ABAQUS/EXPLICIT 6.8-3 on Clemson University’s Palmetto Cluster, a shared computing infrastructure operating at 66 teraFLOPS (trillion floating point operations per second). Each node has at least 2.3 GHz x2 processors (8 cores each) and 12 GB RAM. The soil was modeled using reduced-integration linear brick continuum elements (C3D8R), each being approximately 28 mm on a side (size selected based on the
reference case), except where noted. The models presented here were run on 2 nodes of the cluster and completion times ranged from only a few minutes to about 50 hours, depending primarily on the number of elements in the model.

A built-in algorithm was used to estimate the stable time increment automatically. In ABAQUS/Explicit, automatic time incrementation starts a simulation using element-by-element estimation of the stability limit, which provides a conservative estimate of the true limit. This estimation method computes the natural frequencies of every individual element in the model and uses the highest frequency to compute the time increment. A more accurate global-frequency-based estimate is used only when it will provide a significant advantage in efficiency [21].

6.3.2. Kinematics

For computational efficiency, a symmetry condition is set up at the center of the wheel in the xy-plane (normal to the wheel axis); the nodes initially in the plane are forced to remain in the plane throughout the simulation, and only half of the soil and half of the wheel are modeled. Despite the typical skew-symmetric construction and tread of tires, this simplification is considered reasonable because the soil domain sizing method focuses primarily on the motion of the soil farthest away from the wheel (rigid and without tread in this work). Even for a skew-symmetric pneumatic tire, though, it is likely that the motion of the distant soil would be essentially the same on either side of a lone tire. The bottom of the soil bed and three remaining sides are constrained to zero velocity in all directions, i.e., the nodes are pinned.
The wheel itself is modeled as having negligible mass and moment of inertia. At the center of the wheel on the plane of symmetry, a point-mass is added to represent the mass of the vehicle. The actual values used for these parameters are listed respectively for each case in the tables in Section 5. The cross hatched portion of the surface in Figure 6.2 indicates the 200 mm wide strip along the top of the soil where possible contact is defined between the wheel and the soil. The wheel used in this study is defined as a driving wheel such that only angular velocity is imposed. Slip is allowed, but not prescribed. Any forward motion of the wheel is the result of traction established between the wheel and the soil.

At the wheel-soil interface, a friction coefficient of 0.4 is assumed. Contact between the wheel and the soil was modeled as a contact pair, with the wheel as master and the soil as slave surface. Surface-to-surface contact was used with the penalty
contact method and finite sliding formulation. The contact properties were defined as hard contact with friction, having both the normal and tangential behaviors computed by the penalty method. For this situation (hard contact enforced by the penalty method), ABAQUS/Explicit minimizes penetration of slave nodes into the master surface. The algorithm treats hard contact using a linear stiffness behavior with the stiffness value being automatically adjusted to maintain efficiency. For further details on mechanical contact interactions in ABAQUS/Explicit, see [21].

6.3.3. Adjustment of soil domain sizing method for terrestrial application

In the previous work by Orr, et. al., gravitational loading was applied to the soil and the wheel simultaneously because soil displacement due to self-weight was negligible in the lunar environment [2]. The current work obtained unusable results when following the original procedure as a result of excessive soil settling due to self-weight under earth gravity, particularly in deeper soil beds. In such situations, soil displacement due to self-weight was nearly uniform for a given elevation, and was as much as 2mm at the top surface (Figure 6.3). This displacement caused the soil domain sizing method to fail since it was well above the accuracy limit of 0.1mm at any position on the top surface, making it impossible to satisfy the condition for exiting the iterative expansion step. Therefore it was found necessary to isolate the effect of self-weight by applying gravitational loading to the soil first and allowing it to fully respond prior to introducing any wheel effects into the soil. Then in order to execute the logical tests for the method, the soil displacement was corrected for settling due to self-weight to obtain the actual effect that the wheel had on the soil by subtracting the nodal displacements after settling.
due to self-weight from the nodal displacements at the end of the simulation. With this adjustment, the method was able to be used for the terrestrial simulations without further difficulty. All contour plots subsequent to Figure 6.3 portray corrected nodal displacements.

![Figure 6.3: Contour plots of total (left) and corrected (right) soil displacement after expansion step, demonstrating the need for this correction in order for the reduction step to occur. Note that black indicates displacement magnitude less than accuracy limit of 0.1mm.](image)

6.3.4. Loading

Self-weight due to gravity (9.81 m/s²) was applied to the soil first. The magnitude due to gravity was ramped up smoothly over ten seconds and then held for two seconds to allow the transient response to fade. During this step, the wheel hub remained pinned at its original location. Once the soil’s dynamic response to gravity was complete, and the wheel’s vertical zero-velocity boundary condition was replaced with an upward point force at the hub equal to the wheel load. This external support force was then ramped down to zero smoothly over a period of ten seconds, allowing the full load of the wheel to rest on the soil surface. Again a two-second period was allowed for the system transient response to decay. Finally an angular velocity boundary condition was applied to the
wheel about its axis of rotation. The angular velocity was smoothly ramped from zero to a value equivalent to 0.513 kph on a rigid surface with no slip, based on the wheel’s diameter. This took place over a ten-second period followed by five seconds of constant angular velocity. The smooth angular velocity ramp (and all the other smooth ramps in this study) is a fifth-order polynomial in time, which makes the angular acceleration a fourth-order polynomial with a peak value of 1.88 times the average angular acceleration (Figure 6.4) [4]. The end of the five seconds of constant angular velocity concluded the simulation.

![Smooth Step: Angular Velocity](image)

![Smooth Step: Angular Acceleration](image)

Figure 6.4: Example Wheel Kinematics during Rotation Step for a 500mm Diameter Wheel

6.3.5. Soil Model

The standard soil for this study is a mixture of sands called GRC-1, a highly frictional soil originally developed to simulate the strength properties of lunar regolith [22]. This soil was chosen for convenience and was used in every case except where noted, because it was used in the original proposal of the soil domain sizing method [2]. A later section demonstrates the applicability of the method to other soil types. All soils
in this work are modeled with the Drucker-Prager yield criterion and Cap Plasticity. The Drucker-Prager parameters were calculated from Mohr-Coulomb parameters for the soils chosen using equations (6.1) and (6.2).

\[
\tan \beta = \frac{6 \sin \phi}{3 + \sin \phi} \quad (6.1)
\]

\[
d = \frac{6c \cos \phi}{3 + \sin \phi} \quad (6.2)
\]

The mechanical properties shown in Table 6.1 were used throughout this study except where otherwise indicated.

Table 6.1: Soil Model Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Density [23]</strong></td>
<td></td>
</tr>
<tr>
<td>Bulk Density (g/cm(^3))</td>
<td>1.50</td>
</tr>
<tr>
<td><strong>Elastic [24]</strong></td>
<td></td>
</tr>
<tr>
<td>Young’s Modulus (MPa)</td>
<td>182</td>
</tr>
<tr>
<td>Poisson’s Ratio</td>
<td>0.3</td>
</tr>
<tr>
<td><strong>Mohr-Coulomb Shear Strength [23]</strong></td>
<td></td>
</tr>
<tr>
<td>Cohesion (kPa)</td>
<td>0.90</td>
</tr>
<tr>
<td>Friction Angle (degrees)</td>
<td>46</td>
</tr>
<tr>
<td><strong>Drucker-Prager Shear Strength [23]</strong></td>
<td></td>
</tr>
<tr>
<td>(computed from Mohr-Coulomb values)</td>
<td></td>
</tr>
<tr>
<td>Cohesion (kPa)</td>
<td>1.01</td>
</tr>
<tr>
<td>Friction Angle (degrees)</td>
<td>49.2</td>
</tr>
<tr>
<td><strong>Cap Plasticity [24]</strong></td>
<td></td>
</tr>
<tr>
<td>Cap Eccentricity Parameter</td>
<td>0.4</td>
</tr>
<tr>
<td>Initial Cap Yield Surface Position</td>
<td>0</td>
</tr>
<tr>
<td>Transition Surface Radius Parameter</td>
<td>0.05</td>
</tr>
<tr>
<td>Flow Stress Ratio (K)</td>
<td>1</td>
</tr>
</tbody>
</table>
The cap hardening behavior is modeled according to equation (6.3) using the GRC-1 values of \( C_c = 0.02 \) and \( C_s = 0.005 \) with the initial void ratio equal to 0.5316 at \( p = 6.9 \) kPa [2].

\[
\varepsilon^p_{vol} = \frac{C_c - C_s}{2.3(1 + e_0)} \ln \left( \frac{p}{p_0} \right)
\]  \hspace{1cm} (6.3)

6.4. Methods

The soil domain sizing method has been applied to a variety of systems. The effectiveness of the method is assessed for each system by comparing wheel motion in two simulations with the method-recommended soil domain dimensions: one simulation having the standard pinned boundaries and the other having all roller boundaries instead, as mentioned in Section 3. Further, the influence of different system characteristics on the motion of the wheel is examined by comparing the systems to a reference system. It is important to note that the values listed in the tables throughout this section for wheel load, width, and ratio apply to the whole wheel rather than to simply the half wheel included in the model. In the figures throughout the rest of this paper, the wheel is rolling from left to right. Figure 6.5 and Figure 6.6 illustrate the meaning of symbols used throughout the rest of the paper to evaluate the method and to compare systems, and provide three-dimensional perspective since the results are subsequently presented using two-dimensional views.
Figure 6.5: Definition of symbols used to describe soil dimensions (left) and 3-D contour plot of a typical deformed system (right)

Figure 6.6: Definition of symbols used to describe wheel displacement from starting position. Left depicts wheel prior to rotation; right depicts after rotation.
6.5. Results

Each of the following sub-sections describes the effect of a single system parameter on the effectiveness of the soil domain sizing method and on the motion of the wheel in comparison to the reference case. For each sub-section, a table is given to show the parameter values and the outcomes for each case, including the reference case for comparison. A figure is also given for each sub-section to pictorially illustrate the data contained in the tables.

6.5.1. Effect of wheel load

To evaluate whether the soil domain sizing method works with different wheel loads, two alternative systems were simulated, one with a heavier load and one with a lighter load than the reference case. These results are compared to the reference case in Table 6.2 and Figure 6.7, where it can be seen that the method was successful according to the criteria described previously. The final soil bed dimensions recommended by the method are also given in the table. As expected, the distance behind wheel (B), half-width (C), and depth (D) trend upward with increasing load. The distance ahead of wheel (A) does not keep with the same trend, but the reason is clear when considering the distances traveled (h) in each case. The wheel with the heavier load traveled less distance horizontally due to sinking/slippage. So even though this case produced the smallest value for Dimension A, the difference between Dimension A and the distance traveled (h) for each case reveals that the heavier wheel displaced soil that was more distant from its final location.
### Table 6.2: Results and Evaluation of the Method with Different Wheel Loads

<table>
<thead>
<tr>
<th>Constant Wheel Dimensions</th>
<th>Case 1</th>
<th>Ref.</th>
<th>Case 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>System Values</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>proportion (d/w)</td>
<td>3.33</td>
<td>3.33</td>
<td>3.33</td>
</tr>
<tr>
<td>diameter (mm)</td>
<td>500</td>
<td>500</td>
<td>500</td>
</tr>
<tr>
<td>width (mm)</td>
<td>150</td>
<td>150</td>
<td>150</td>
</tr>
<tr>
<td>load (kg)</td>
<td>110</td>
<td>184</td>
<td>306</td>
</tr>
<tr>
<td>Final Soil Domain</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dimensions (mm)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dimensions (mm)</td>
<td>A</td>
<td>1850</td>
<td>1900</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>210</td>
<td>300</td>
</tr>
<tr>
<td></td>
<td>C</td>
<td>390</td>
<td>460</td>
</tr>
<tr>
<td></td>
<td>D</td>
<td>300</td>
<td>470</td>
</tr>
<tr>
<td>Wheel Displ. (pinned BC)</td>
<td>g:</td>
<td>6.6</td>
<td>12.3</td>
</tr>
<tr>
<td></td>
<td>h:</td>
<td>1487</td>
<td>1444</td>
</tr>
<tr>
<td></td>
<td>v:</td>
<td>11.2</td>
<td>23.1</td>
</tr>
<tr>
<td>Wheel Displ. (sliding BC)</td>
<td>g:</td>
<td>6.3</td>
<td>12.0</td>
</tr>
<tr>
<td></td>
<td>h:</td>
<td>1487</td>
<td>1444</td>
</tr>
<tr>
<td></td>
<td>v:</td>
<td>11.4</td>
<td>23.4</td>
</tr>
<tr>
<td>% difference (pinned vs.</td>
<td>Δg/g:</td>
<td>-3.97</td>
<td>-2.20</td>
</tr>
<tr>
<td>sliding)</td>
<td>Δh/h:</td>
<td>-0.01</td>
<td>-0.05</td>
</tr>
<tr>
<td></td>
<td>Δv/v:</td>
<td>1.51</td>
<td>1.26</td>
</tr>
</tbody>
</table>
6.5.2. Effect of Wheel Size

In order to demonstrate that the soil domain sizing method is applicable for wheels of different size, a set of simulations was performed with the wheel load and wheel ratio (diameter/width) held constant. Without adjustment, the method produced an appropriate soil size for all these cases except the 250mm wheel case (Case 3a). In that case the relatively small wheel sunk into the soil excessively, and the final wheel position was not independent of boundary conditions. However this simulation was repeated using a finer mesh (Case 3b) and produced a wheel response that was independent of boundary conditions. Despite large differences in the wheel motion between Case 3a and
Case 3b, the sets of soil dimensions recommended by the method for both cases were similar. In Figure 6.8 (Case 3a), the insufficiency of the coarser 28mm mesh is visible around bottom of the wheel; only about four linear elements form the soil boundary that contacts the wheel. The finer 20mm mesh has about six elements in contact (Figure 6.8, Case 3bFigure 6.9) and makes a smoother approximation to the arc for this large of an angle. This observation is consistent with what will be seen in a later section (Case 8, Figure 6.9), where a deep-sinking wheel of larger diameter does not need a finer mesh despite a large angle of contact since there is a larger number of elements in contact along the arc of the wheel. Table 6.3 contains the values corresponding to the simulations pictured in Figure 6.8.

Cases 3a and 3b brought to light an opportunity for an adaptation to the soil-sizing method. Since in this situation the wheel did not travel nearly as far as predicted by the rigid wheel/rigid surface estimate during the initial step, and because the significant soil displacement did not approach the soil boundary ahead of the wheel (significant displacement ends at 670mm with soil dimension A equal to 2200mm for this step), it was concluded that the soil box could be shortened significantly in the direction of travel even prior to the expansion step. The method as originally proposed would have required that dimension A be left intact at 2200mm for the expansion step. But the purpose of the expansion step is to produce a soil box much larger than needed (as defined by significant displacement at least a characteristic length from any boundary). Therefore, in keeping with this purpose and to avoid over-trimming, the dimension A was reduced such that the boundary was still roughly two characteristic lengths beyond the significant soil
displacement as observed in the initial step (i.e. dimension A equal to 670mm + 2(250mm) = 1170mm for the expansion step). This allowed sufficient material to meet the exit criteria for the expansion step loop while avoiding simulation of an excessive amount of material that had already been shown to be insignificant.

Also noteworthy is the behavior of the largest wheel (Case 5), which demonstrated a unique behavior among all the cases simulated in this work. As it began to travel, it climbed to a higher vertical position (v is less than g); all other cases sank deeper during rotation. However, considering the lightness of the load relative to wheel size [14], it is intuitively not surprising that the wheel demonstrated this behavior.

Table 6.3: Results and Evaluation of Method with Different Wheel Sizes

<table>
<thead>
<tr>
<th>Constant wheel load</th>
<th>Case 3a</th>
<th>Case 3b*</th>
<th>Case 4</th>
<th>Ref.</th>
<th>Case 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>System Values</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>proportion (d/w)</td>
<td>3.33</td>
<td>3.33</td>
<td>3.33</td>
<td>3.33</td>
<td>3.33</td>
</tr>
<tr>
<td>diameter (mm)</td>
<td>250</td>
<td>250</td>
<td>400</td>
<td>500</td>
<td>1000</td>
</tr>
<tr>
<td>width (mm)</td>
<td>75</td>
<td>75</td>
<td>120</td>
<td>150</td>
<td>300</td>
</tr>
<tr>
<td>load (kg)</td>
<td>184</td>
<td>184</td>
<td>184</td>
<td>184</td>
<td>184</td>
</tr>
<tr>
<td>Final Soil Domain Dimensions (mm)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>670</td>
<td>650</td>
<td>1310</td>
<td>1900</td>
<td>1840</td>
</tr>
<tr>
<td>B</td>
<td>380</td>
<td>400</td>
<td>300</td>
<td>300</td>
<td>190</td>
</tr>
<tr>
<td>C</td>
<td>460</td>
<td>450</td>
<td>490</td>
<td>460</td>
<td>410</td>
</tr>
<tr>
<td>D</td>
<td>490</td>
<td>500</td>
<td>480</td>
<td>470</td>
<td>420</td>
</tr>
<tr>
<td>Wheel Displ. (pinned BC) (mm)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>g:</td>
<td>36.6</td>
<td>52.2</td>
<td>13.9</td>
<td>12.3</td>
<td>3.9</td>
</tr>
<tr>
<td>h:</td>
<td>141</td>
<td>115</td>
<td>792</td>
<td>1444</td>
<td>1502</td>
</tr>
<tr>
<td>v:</td>
<td>84.0</td>
<td>100.8</td>
<td>54.1</td>
<td>23</td>
<td>3.0</td>
</tr>
<tr>
<td>Wheel Displ. (sliding BC) (mm)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>g:</td>
<td>36.8</td>
<td>52.1</td>
<td>14.3</td>
<td>12.0</td>
<td>4.1</td>
</tr>
<tr>
<td>h:</td>
<td>118</td>
<td>115</td>
<td>780</td>
<td>1444</td>
<td>1501</td>
</tr>
<tr>
<td>v:</td>
<td>72.7</td>
<td>101.7</td>
<td>54.2</td>
<td>23.4</td>
<td>3.2</td>
</tr>
<tr>
<td>% difference</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Δg/g:</td>
<td>0.60</td>
<td>-0.19</td>
<td>3.09</td>
<td>-2.20</td>
<td>6.85</td>
</tr>
<tr>
<td>Δh/h:</td>
<td>-16.67</td>
<td>-0.05</td>
<td>-1.62</td>
<td>-0.05</td>
<td>-0.03</td>
</tr>
<tr>
<td>Δw/v:</td>
<td>-13.45</td>
<td>0.90</td>
<td>0.16</td>
<td>1.26</td>
<td>4.42</td>
</tr>
</tbody>
</table>

*Mesh element size: 20mm on a side
Figure 6.8: Depiction of Final Soil Domain Sizes with different wheel sizes
6.5.3. Effect of Wheel Ratio

In order to evaluate whether varying wheel ratio (diameter/width) causes difficulty for the soil domain sizing method, simulations were performed with wheels of different widths but all having the same diameter. Table 6.4 and Figure 6.9 contain these results, which demonstrate that the method is applicable to these systems. It is noted that Case 8, wheel ratio equal to 10, returned an exceptionally low value of horizontal travel. This can easily be seen to be the result of excessive sinking (Figure 6.9) which led to excessive wheel slippage and loss of mobility. Review of the data shows that the wheel had already reached within 0.5mm of its final horizontal position after twelve seconds of rotation; during the final three seconds the wheel was essentially operating at 100 percent slip. Still, the method returned a final soil size that was appropriate for this particular case without mesh refinement.
Table 6.4: Results and Evaluation of Method with Different Wheel Ratios

<table>
<thead>
<tr>
<th>Constant wheel load</th>
<th>Case 6</th>
<th>Ref.</th>
<th>Case 7</th>
<th>Case 8</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>System Values</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>proportion (d/w)</td>
<td>2</td>
<td>3.33</td>
<td>5.56</td>
<td>10</td>
</tr>
<tr>
<td>diameter (mm)</td>
<td>500</td>
<td>500</td>
<td>500</td>
<td>500</td>
</tr>
<tr>
<td>width (mm)</td>
<td>250</td>
<td>150</td>
<td>90</td>
<td>50</td>
</tr>
<tr>
<td>load (kg)</td>
<td>184</td>
<td>184</td>
<td>184</td>
<td>184</td>
</tr>
<tr>
<td><strong>Final Soil Domain</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dimensions (mm)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>1890</td>
<td>1900</td>
<td>1850</td>
<td>950</td>
</tr>
<tr>
<td>B</td>
<td>210</td>
<td>300</td>
<td>350</td>
<td>400</td>
</tr>
<tr>
<td>C</td>
<td>440</td>
<td>460</td>
<td>480</td>
<td>450</td>
</tr>
<tr>
<td>D</td>
<td>440</td>
<td>470</td>
<td>480</td>
<td>470</td>
</tr>
<tr>
<td><strong>Wheel Displ. (pinned BC)</strong> (mm)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>g:</td>
<td>6.3</td>
<td>12.3</td>
<td>22.3</td>
<td>73.6</td>
</tr>
<tr>
<td>h:</td>
<td>1503</td>
<td>1444</td>
<td>1350</td>
<td>407</td>
</tr>
<tr>
<td>v:</td>
<td>7.9</td>
<td>23.1</td>
<td>44.8</td>
<td>127</td>
</tr>
<tr>
<td><strong>Wheel Displ. (sliding BC)</strong> (mm)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>g:</td>
<td>6.7</td>
<td>12.0</td>
<td>23.4</td>
<td>73.4</td>
</tr>
<tr>
<td>h:</td>
<td>1502</td>
<td>1444</td>
<td>1349</td>
<td>406</td>
</tr>
<tr>
<td>v:</td>
<td>8.1</td>
<td>23.4</td>
<td>45.1</td>
<td>125</td>
</tr>
<tr>
<td><strong>% difference</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>∆g/g:</td>
<td>6.23</td>
<td>-2.20</td>
<td>4.54</td>
<td>-0.24</td>
</tr>
<tr>
<td>∆h/h:</td>
<td>-0.06</td>
<td>-0.05</td>
<td>-0.05</td>
<td>-0.31</td>
</tr>
<tr>
<td>∆v/v:</td>
<td>2.28</td>
<td>1.26</td>
<td>0.62</td>
<td>-1.96</td>
</tr>
</tbody>
</table>
6.5.4. Effect of soil type

The soil domain sizing method was originally developed for traction simulation studies using the specific type of soil that is encountered on the lunar surface. All cases presented up to this point have used soil properties obtained from a simulant of lunar soil, which is a sand of unusually high friction angle. Therefore it is important to evaluate the
performance of the method on soil types typical of a terrestrial environment. Two soils have been chosen, a typical sand and a typical soft saturated clay. The Young’s modulus, soil cohesion, and friction angle have been modified in the simulation; all other soil properties have been left the same as those reported in Table 6.1 since they are within range for realistic earth soils [18]. Also all wheel properties have been left the same as those reported previously for the reference case. From Table 6.5 and Figure 6.10 it can be seen that the sand used in Case 9 demonstrated a need for a much deeper soil box than had been seen in the reference case, while the clay of Case 10 required an exceptionally wide box. Neither terrestrial soil allowed the wheel to travel as far horizontally as the reference lunar soil allowed, attributable to the exceptionally high friction angle resulting from highly angular grains comprising the lunar soil. Clearly for use on these terrestrial soils, a larger diameter (and/or wider) wheel would be required to reduce slip and sinkage and to improve mobility. Still, regardless of the tractive performance of the wheel on the given soil, the soil domain sizing method successfully produced a soil box size that allowed wheel travel to be essentially unaffected by boundary condition type.
Table 6.5: Results and Evaluation of Method with Different Soil Types

<table>
<thead>
<tr>
<th>Mohr-Coulomb</th>
<th>Case 9</th>
<th>Ref.</th>
<th>Case 10</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soil Type</td>
<td>sand</td>
<td>GRC</td>
<td>clay</td>
</tr>
<tr>
<td>Young's mod (MPa)</td>
<td>30 (13)</td>
<td>182</td>
<td>5 (13)</td>
</tr>
<tr>
<td>Cohesion (kPa)</td>
<td>*0.674</td>
<td>0.9</td>
<td>9.5 (13)</td>
</tr>
<tr>
<td>Friction Angle</td>
<td>30° (13)</td>
<td>46°</td>
<td>*0.0005°</td>
</tr>
<tr>
<td>Final Soil Domain Dimensions</td>
<td>mm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>800</td>
<td>1850</td>
<td>1710</td>
</tr>
<tr>
<td>B</td>
<td>470</td>
<td>350</td>
<td>550</td>
</tr>
<tr>
<td>C</td>
<td>500</td>
<td>480</td>
<td>980</td>
</tr>
<tr>
<td>D</td>
<td>640</td>
<td>480</td>
<td>580</td>
</tr>
<tr>
<td>Wheel Displ. (pinned BC)</td>
<td>mm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>g:</td>
<td>44.6</td>
<td>12.3</td>
<td>24.4</td>
</tr>
<tr>
<td>h:</td>
<td>208</td>
<td>1444</td>
<td>1043</td>
</tr>
<tr>
<td>v:</td>
<td>85.7</td>
<td>23.1</td>
<td>37.1</td>
</tr>
<tr>
<td>Wheel Displ. (sliding BC)</td>
<td>mm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>g:</td>
<td>44.1</td>
<td>12.0</td>
<td>24.4</td>
</tr>
<tr>
<td>h:</td>
<td>210</td>
<td>1444</td>
<td>1040</td>
</tr>
<tr>
<td>v:</td>
<td>86.0</td>
<td>23.4</td>
<td>37.1</td>
</tr>
<tr>
<td>% difference</td>
<td>Δg/g:</td>
<td>-1.17</td>
<td>-2.20</td>
</tr>
<tr>
<td></td>
<td>Δh/h:</td>
<td>1.25</td>
<td>-0.05</td>
</tr>
<tr>
<td></td>
<td>Δv/v:</td>
<td>0.36</td>
<td>1.26</td>
</tr>
</tbody>
</table>

*Cohesion for sand and friction angle for clay were selected as the lowest values that did not cause errors in the simulation*
6.6. Conclusions and Recommendations

From all the data presented thus far, it is clear that the variation of dimensions and loads associated with a wheel can have a tremendous effect on the outcome of the simulation. Factors that are affected include position of the wheel at different times, speed of the wheel at different times, and displacement of the soil at different positions. Furthermore, variations in the soil type influence these factors as well. In all cases, the amount of soil required for an accurate model (or physical experiment for that matter) is likely to be different, and should be determined independently for each case, or possibly
for a group of similar cases. It has been demonstrated in this work that the method to select soil domain dimensions for a dynamic wheel-soil model is capable of selecting appropriate dimensions in all of these cases. However it was seen that caution must be exercised when making seemingly minor system changes (e.g. increased wheel load/sinkage) that may influence the adequacy of mesh refinement or otherwise affect the accuracy of the simulation. Additionally, it was recognized that the method could be made more efficient for cases of high wheel slippage resulting in low travel because in such cases the dimension A of the soil could be “pre-reduced” before the expansion step. The value recommended for this pre-reduction was two characteristic lengths beyond any significant soil displacement observed in the initialization step.
7. CONCLUSIONS AND FUTURE WORK

7.1. Conclusions

A large amount of data from two-dimensional DEM simulations of the Direct Shear Test was collected and was analyzed. The data was used to gain understanding of the influence of each DEM parameter on the shear strength of a DEM soil specimen. This understanding makes it possible to calibrate a DEM model through trial and error, by repeatedly adjusting the parameters known to affect the desired outcomes. Further, a set of equations was developed by statistical modeling techniques such that appropriate model parameters can be selected directly, based on desired friction angles of peak stress and residual stress. The direct selection process was carried out using a certain type of sand (“MGR sand”) and was checked against experimental DST results of that sand. The WEST-MGRS system was used to collect physical data about the tractive performance of six different grouser configurations on a rigid wheel in the MGR sand; the experiment was reproduced in simulation using the calibrated DEM model. Finally, the Orr soil domain sizing method was evaluated for versatility by applying the method to a variety of different wheel/soil systems using FEM. A summary of the research questions addressed by this work, with their answers, is given in Table 7.1.
Table 7.1: Research Questions with answers.

<table>
<thead>
<tr>
<th>RQ1</th>
<th>How do the modeling parameters of friction coefficient, dyad eccentricity, normal contact stiffness, shear contact stiffness, porosity, rate of shear, and upscale factor influence the shear strength of a simulated sand in DEM?</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Each parameter influences the shear strength differently; friction coefficient and dyad eccentricity have the greatest effect. Plots demonstrating the effect of each parameter are given in Section 4.2.1.</td>
</tr>
<tr>
<td>RQ2</td>
<td>Can a large body of data collected from simulations using a variety of DEM parameters be used to fit a statistical model that will enable the direct selection of appropriate parameters to achieve specific desired system behavior?</td>
</tr>
<tr>
<td></td>
<td>Yes, such a model of the data has been developed and has been used with good results on a test case, as described in Section 4.2.3.</td>
</tr>
<tr>
<td>RQ3</td>
<td>Can a 2-D wheel/soil model in DEM be used to compare the performance of different grouser configurations and predict which one(s) will develop superior traction in sand?</td>
</tr>
<tr>
<td></td>
<td>A 2-D wheel/soil model was developed in DEM to simulate the behavior of the MGR testing system. As expected, the model did not accurately predict the actual acceleration value realized by the physical system because of 3-D effects; however it did provide an accurate prediction of how the different grouser configurations compared to each other, i.e. which was best, second-best, etc. The results of the wheel/soil simulations are described in Section 5.2.</td>
</tr>
<tr>
<td>RQ4</td>
<td>Does the soil sizing method proposed by Orr work for a wide variety of systems?</td>
</tr>
<tr>
<td></td>
<td>The method for selecting soil domain dimensions was tested with varying wheel geometries, wheel loads, and soil types. With minor adjustments to account for gravitational conditions of the environment (i.e. earth vs. moon) and for cases of limited wheel travel due to excessive slip, the method was found to prescribe reasonable soil dimensions for all the cases tested. Details are available in Section 6.</td>
</tr>
</tbody>
</table>
7.2. Future Work

Many opportunities exist for continuation of the research presented in this
document. A few of them are mentioned and discussed here.

7.2.1. Effects of Additional Parameters on Strength in Two Dimensions

The parameters of friction coefficient, particle eccentricity, contact stiffness, and
porosity have been studied in this work, in terms of their effects on shear strength. The
effect of damping coefficient has not been examined at all. A study of its influence in the
model would be of merit, particularly in cases where high relative speeds exist between
particles, such as in the case of a wheel “burning out” or slipping at a high rate. As
mentioned in Chapter 5, the damping coefficient may be strongly influencing the
prediction of rolling resistance; this possibility in particular should be investigated.
Additionally, no particle shape has been studied besides dyads (and rounds); the
examination of other shapes likely would result in improved models.

7.2.2. Coupled FEM/DEM Simulation in Two Dimensions

The calibrated 2-D DEM model can be integrated into a coupled FEM/DEM
model of the problem in two dimensions. Although coupled FEM/DEM models have
been implemented in the past, most appear to be rather simplistic, particularly regarding
the way they handle the interface between boundaries of the FEM and DEM domains.
The boundaries need to be designed so as not to create an abrupt, straight-line border;
rather, the border should consist of a transitional layer that has attributes of both the FEM
and the DEM segments. Done correctly, the coupling should be performed so as to
model the wheel (rigid or deformable) with FEM. The soil should be modeled with DEM
in the regions near the wheel because these experience the most extreme shear strains; all other soil regions should be modeled using FEM. Such a coupled model would offer “the best of both worlds,” that is, the granular representation of matter available in a DEM model along with the ability to model large domains using FEM.

7.2.3. Three-Dimensional Wheel/Soil Simulation in DEM

Perhaps the most important next step for this research is a 3-D study of parameter effects on shear strength in DEM models. Such a study would require a great deal of computational resources and would be infeasible without a DEM code capable of extreme parallelization. Such a code is expensive to purchase commercially; therefore writing a custom code is recommended. Some aspects of this task are discussed in the following subsections.

7.2.3.1. Description of Primary Code Modules

The basic calculation cycle of DEM as discussed in Chapter 3 provides an indication of the primary operations that must be effected by the code. The Force module takes the current state of the model (position and velocity of each element, contact properties) and sends this information to the contact detection algorithm. The contact detection algorithm operates as a subroutine of the Force module and is responsible for defining cell space, searching for contact, and computing overlap quantities and relative velocities between particles in contact. The Force module then uses these results to compute the sum of forces acting on every element, and knowing the mass and the inertia tensor of each element, determines the acceleration components (linear and angular) of each element. Another subroutine (Time step subroutine) takes the mass and stiffness
data associated with each element and computes the natural vibration frequency of the element; the element with the highest frequency determines the maximum stable time increment for the integration. The acceleration components and the time increment are returned to the master program. At this point, the program sends the acceleration data to the Integration module, along with the current element positions and velocities. The Integration module performs explicit time integration, wherein the current state of the model is advanced to the next time increment by determining first the new velocity of each element and then each element’s position. Then the cycle may be repeated.

7.2.3.2. Potential Challenges

The challenges associated with the production of a custom 3-D DEM code are related more to the knowledge and experience of the programmer than to problems that have not yet been solved, because others have written similar codes. From the perspective of the author, some of the most significant challenges include defining and adaptively redefining the cell space for contact search. This task is important mainly for efficiency of the code’s operation. Also, the proper allocation of memory and the referencing of items through linked lists as described in [15] is an important challenge. Finally, the most important challenge is the implementation of parallel computing into the code because without this feature, even the best-written 3-D code will be useless since it cannot obtain results in a reasonable amount of time.
7.2.4. *Coupled FEM/DEM Simulation in Three Dimensions*

Once a 3-D model in DEM is available and information is generated regarding the selection of 3-D soil parameters, steps should be taken to couple the 3-D DEM model with a 3-D FEM model (Figure 7.1). Such a model should be implemented in a similar fashion as previously described for the coupled 2-D model. When complete, this model will be able to provide highly accurate results for a wide variety of wheel/soil situations.

Figure 7.1: Recommended future simulation implementing coupled FEM/DEM model in 3-D.
A. Derivation of Equation 3.3

Figure A.1: Representative differential element for derivation of Equation 3.3.

Referring to Figure A.1, consider a collection of circular (2-D) particles with randomly-generated radii between the values of $r_{\text{min}}$ and $r_{\text{max}}$, and having a uniform probability density. The area beneath the distribution is divided into $B$ equal regions, each of width $\Delta r$. Thus the number of regions $B$ is equal to:

$$B = \frac{r_{\text{max}} - r_{\text{min}}}{\Delta r} \quad (A.1)$$

If the total number of particles is $n$, the number of particles in a given region is:

$$n_i = \frac{n}{B} = \frac{n\Delta r}{r_{\text{max}} - r_{\text{min}}} \quad (A.2)$$

Each region represents a range of radii close to $r_i$. Because the probability density is uniform and because the widths are equal, each region is expected to represent the same
number of particles, \(n_i\). The area occupied by the circular particles in one region is approximately:

\[
A_i = n_i (\pi r_i^2) = \frac{n \Delta r}{r_{\text{max}} - r_{\text{min}}} (\pi r_i^2) \quad (A.3)
\]

The total area \(A_p\) occupied by particles in the system then is:

\[
A_p = \sum_{i=1}^{B} A_i = \sum_{i=1}^{B} \frac{n}{r_{\text{max}} - r_{\text{min}}} (\pi r_i^2) \Delta r \quad (A.4)
\]

Then in the limiting case, as the width of the regions goes to zero, \(B\) goes to infinity, and the result is:

\[
A_p = \int_{r_{\text{min}}}^{r_{\text{max}}} \frac{n}{r_{\text{max}} - r_{\text{min}}} (\pi r^2) dr \quad (A.5)
\]

The constant values are brought outside the integral and the integral is evaluated:

\[
A_p = \frac{n \pi}{r_{\text{max}} - r_{\text{min}}} \int_{r_{\text{min}}}^{r_{\text{max}}} (r^2) dr = \frac{n \pi (r_{\text{max}}^3 - r_{\text{min}}^3)}{3(r_{\text{max}} - r_{\text{min}})} \quad (A.6)
\]

If the ratio of maximum to minimum radii in the system is defined as \(F\), then:

\[
r_{\text{max}} = Fr_{\text{min}} \quad (A.7)
\]

And Equation (A.6) simplifies to

\[
A_p = \frac{n\pi r_{\text{min}}^2 (F^3 - 1)}{3(F - 1)} \quad (A.8)
\]

Accounting for the porosity (\(\eta\)), the total area \(A\) occupied by material \((A_p)\) and void \((A_v)\) is

\[
A = A_p + A_v \quad (A.9)
\]

or, equivalently,
\[ A_p = A - A_v = A - \eta A = A(1 - \eta) \quad (A.10) \]

Combining Equations (A.8) and (A.10), the final result is Equation (A.11), which can be solved for \( r_{\text{min}} \) to obtain Equation (3.3), which uses the symbols \( n_{\text{balls}} \) and \( \eta_{\text{target}} \) instead of \( n \) and \( \eta \), respectively.

\[ A(1 - \eta) = \frac{n\pi r_{\text{min}}^2(F^3 - 1)}{3(F - 1)} \quad (A.11) \]
B. Values used to generate bar charts in Chapter 4.

Table A.1: Values used to generate Figure 4.16.

<table>
<thead>
<tr>
<th></th>
<th>Friction Angle: residual</th>
<th>Friction Angle: peak</th>
</tr>
</thead>
<tbody>
<tr>
<td>MGR sand actual value</td>
<td>32.5°</td>
<td>39.0°</td>
</tr>
<tr>
<td>Case 1 predicted lower limit</td>
<td>27.6°</td>
<td>25.8°</td>
</tr>
<tr>
<td>Case 1 actual values:</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>34.7°</td>
<td>37.2°</td>
</tr>
<tr>
<td></td>
<td>35.4°</td>
<td>40.0°</td>
</tr>
<tr>
<td></td>
<td>29.8°</td>
<td>38.5°</td>
</tr>
<tr>
<td></td>
<td>33.7°</td>
<td>40.5°</td>
</tr>
<tr>
<td></td>
<td>31.0°</td>
<td>37.5°</td>
</tr>
<tr>
<td></td>
<td>29.7°</td>
<td>35.5°</td>
</tr>
<tr>
<td>Case 1 mean value:</td>
<td>32.4°</td>
<td>38.2°</td>
</tr>
<tr>
<td>Case 1 predicted upper limit</td>
<td>37.3°</td>
<td>52.3°</td>
</tr>
<tr>
<td>Case 2 predicted lower limit</td>
<td>27.7°</td>
<td>25.8°</td>
</tr>
<tr>
<td>Case 2 actual values:</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>30.0°</td>
<td>39.1°</td>
</tr>
<tr>
<td></td>
<td>31.5°</td>
<td>38.2°</td>
</tr>
<tr>
<td></td>
<td>28.1°</td>
<td>37.1°</td>
</tr>
<tr>
<td></td>
<td>31.5°</td>
<td>46.5°</td>
</tr>
<tr>
<td></td>
<td>29.2°</td>
<td>47.6°</td>
</tr>
<tr>
<td></td>
<td>26.0°</td>
<td>32.3°</td>
</tr>
<tr>
<td>case 2 mean value:</td>
<td>29.4°</td>
<td>40.1°</td>
</tr>
<tr>
<td>Case 2 predicted upper limit</td>
<td>37.3°</td>
<td>52.3°</td>
</tr>
</tbody>
</table>
Table A.2: Values used to generate Figure 4.18.

<table>
<thead>
<tr>
<th></th>
<th>Friction Angle: residual</th>
<th>Friction Angle: peak</th>
</tr>
</thead>
<tbody>
<tr>
<td>MGR sand actual value</td>
<td>32.5°</td>
<td>39.0°</td>
</tr>
<tr>
<td>Case 1 predicted lower limit</td>
<td>27.6°</td>
<td>25.8°</td>
</tr>
<tr>
<td>Case 1 actual values, conf.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>pressure 75 kPa</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>29.9°</td>
<td>34.2°</td>
</tr>
<tr>
<td></td>
<td>31.6°</td>
<td>37.6°</td>
</tr>
<tr>
<td></td>
<td>30.4°</td>
<td>34.3°</td>
</tr>
<tr>
<td></td>
<td>32.4°</td>
<td>38.8°</td>
</tr>
<tr>
<td></td>
<td>31.8°</td>
<td>37.7°</td>
</tr>
<tr>
<td>Mean, 75 kPa</td>
<td>31.2°</td>
<td>36.5°</td>
</tr>
<tr>
<td>Case 1 actual values, conf.</td>
<td>28.8°</td>
<td>31.5°</td>
</tr>
<tr>
<td>pressure 150 kPa</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>29.3°</td>
<td>33.2°</td>
</tr>
<tr>
<td></td>
<td>30.5°</td>
<td>32.0°</td>
</tr>
<tr>
<td>Mean, 150 kPa</td>
<td>29.5°</td>
<td>32.2°</td>
</tr>
<tr>
<td>Case 1 actual values, conf.</td>
<td>31.7°</td>
<td>36.3°</td>
</tr>
<tr>
<td>pressure 300 kPa</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>32.5°</td>
<td>35.6°</td>
</tr>
<tr>
<td></td>
<td>29.2°</td>
<td>31.6°</td>
</tr>
<tr>
<td>Mean, 300 kPa</td>
<td>31.1°</td>
<td>34.5°</td>
</tr>
<tr>
<td>Case 1 predicted upper limit</td>
<td>37.3°</td>
<td>52.3°</td>
</tr>
<tr>
<td>Case 2 predicted lower limit</td>
<td>27.7°</td>
<td>25.8°</td>
</tr>
<tr>
<td>Case 2 actual values, conf.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>pressure 75 kPa</td>
<td>26.4°</td>
<td>36.9°</td>
</tr>
<tr>
<td></td>
<td>32.0°</td>
<td>39.4°</td>
</tr>
<tr>
<td></td>
<td>26.0°</td>
<td>33.5°</td>
</tr>
<tr>
<td></td>
<td>31.1°</td>
<td>39.8°</td>
</tr>
<tr>
<td></td>
<td>27.3°</td>
<td>35.7°</td>
</tr>
<tr>
<td>Mean, 75 kPa</td>
<td>28.6°</td>
<td>37.1°</td>
</tr>
<tr>
<td>Case 2 actual values, conf.</td>
<td>28.4°</td>
<td>32.9°</td>
</tr>
<tr>
<td>pressure 150 kPa</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>28.2°</td>
<td>35.4°</td>
</tr>
<tr>
<td></td>
<td>31.1°</td>
<td>34.9°</td>
</tr>
<tr>
<td>Mean, 150 kPa</td>
<td>29.3°</td>
<td>34.4°</td>
</tr>
<tr>
<td>Case 2 actual values, conf.</td>
<td>25.3°</td>
<td>28.9°</td>
</tr>
<tr>
<td>pressure 300 kPa</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>28.8°</td>
<td>32.0°</td>
</tr>
<tr>
<td></td>
<td>27.6°</td>
<td>32.7°</td>
</tr>
<tr>
<td>Mean, 300 kPa</td>
<td>27.2°</td>
<td>31.2°</td>
</tr>
<tr>
<td>Case 2 predicted upper limit</td>
<td>37.3°</td>
<td>52.3°</td>
</tr>
</tbody>
</table>
Table A.3: Values used to generate Figure 4.20.

<table>
<thead>
<tr>
<th></th>
<th>Friction Angle: residual</th>
<th>Friction Angle: peak</th>
</tr>
</thead>
<tbody>
<tr>
<td>MGR sand actual value</td>
<td>32.5°</td>
<td>39.°</td>
</tr>
<tr>
<td>Case 1 predicted lower limit</td>
<td>27.6°</td>
<td>25.8°</td>
</tr>
<tr>
<td>Case 1 actual values, conf.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>pressure 30 kPa</td>
<td>32.3°</td>
<td>38.9°</td>
</tr>
<tr>
<td></td>
<td>31.6°</td>
<td>38.5°</td>
</tr>
<tr>
<td></td>
<td>32.4°</td>
<td>37.3°</td>
</tr>
<tr>
<td>Mean</td>
<td>32.1°</td>
<td>38.3°</td>
</tr>
<tr>
<td>Case 1 predicted upper limit</td>
<td>37.3°</td>
<td>52.3°</td>
</tr>
<tr>
<td>Case 2 predicted lower limit</td>
<td>27.7°</td>
<td>25.8°</td>
</tr>
<tr>
<td>Case 2 actual values, conf.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>pressure 30 kPa</td>
<td>28.9°</td>
<td>38.9°</td>
</tr>
<tr>
<td></td>
<td>30.3°</td>
<td>42.4°</td>
</tr>
<tr>
<td></td>
<td>29.7°</td>
<td>41.4°</td>
</tr>
<tr>
<td>Mean</td>
<td>29.6°</td>
<td>40.9°</td>
</tr>
<tr>
<td>Case 2 predicted upper limit</td>
<td>37.3°</td>
<td>52.3°</td>
</tr>
</tbody>
</table>
C. PFC Simulation Control Codes

Scripts were used to control all simulations in PFC. All scripts are stored in ASCII files; the files are given different file extensions, depending on the functionality of the code in the file. The complete set of scripts follows for the Direct Shear Test and then for the wheel/soil simulations. Each filename is listed first in bold font, followed by the text of the code.

a. Direct Shear Test Codes

Note that by changing the three variables (run_num, press_num, and run_let) in the main driver file for the Direct Shear Test, the parameters of the simulation are automatically selected.

i. ASTM_DST_Equil_Test_001a.dvr

;filename ASTM_DST_Equil_test_001a.dvr

new

def variables
  run_num=00
  press_num=1
  run_let='a'
  fname='ASTM_DST_shear_time_'+'00'+string(press_num)+run_let
  fname2=fname+'_final'
  avi_name1=fname+'compact.avi'
end

variables

set logfile fname
set log on

call case_conditions.dvr
case_conditions

set rand rand_seed

call make_d_shear.dvr

call direct_shear.dvr
print fname
;EOF 'fname'+.dvr

Quit
ii. Case_conditions.dvr

;fname case_conditions.dvr
;selects parameters based on run number and pressure number
;run number xy => property x, property value y
;x=1 => fric, x=2 => Kn, x=3 => Ks, x=4 => shape, x=5 => Shear vel, x=6 => upscale, x=7 => porosity
;y=1 => minimum parameter value, y=2 => next smallest value, etc.
;all other parameters will assume the standard values
;pressure number z => confining pressure = z*75 kPa
;run letter => random specimen id

def case_conditions
;standard conditions
    coef_fric=1
    kn_final=1e8
    ks_final=1e8
    shape_sep=0
    shear_time=1
    USC=1
    por_limit=.15
    if run_num=00
        endif
    if run_num=11
        coef_fric=.1
        endif
    if run_num=12
        coef_fric=.3
        endif
    if run_num=13
        coef_fric=3
        endif
    if run_num=14
        coef_fric=10
        endif
    if run_num=21
        kn_final=3e8
        endif
    if run_num=22
        kn_final=1e9
        endif
    if run_num=31
        ks_final=3e8
        endif
    if run_num=32
        ks_final=1e9
        endif
    if run_num=41
        shape_sep=.5
        endif
    if run_num=42
shape_sep=1
endif
if run_num=43
    shape_sep=1.5
endif
if run_num=44
    shape_sep=2
endif
if run_num=45
    shape_sep=1.5
    coef_fric=3
endif
if run_num=46
    shape_sep=2.5
endif
if run_num=51
    shear_time=.8
endif
if run_num=52
    shear_time=1.2
endif
if run_num=61
    USC=3
endif
if run_num=62
    USC=10
endif
if run_num=71
    por_limit=.14
endif
if run_num=72
    por_limit=.145
endif
if run_num=73
    por_limit=.155
endif
if run_num=74
    por_limit=.16
endif
if run_num=75
    por_limit=.165
endif
if run_num=76
    por_limit=.17
endif
if run_num=77
    por_limit=.175
endif
if run_num=78
    por_limit=.18
endif
if run_num=79
  por_limit=0.185
endif

if run_num=81
  por_limit=0.17
  shape_sep=2
  coef_fric=0.3
endif

if run_num=82
  shape_sep=1.8
endif

if run_num=83
  shape_sep=1.9
  por_limit=0.16
endif

if run_num=84
  shape_sep=1.8
  coef_fric=3
  por_limit=0.165
endif

if run_num=85
  shape_sep=2
  coef_fric=0.6
  por_limit=0.155
endif

if run_num=86
  shape_sep=2
  coef_fric=0.65
  por_limit=0.165
endif

if run_num=87
  shape_sep=2
  coef_fric=0.7
  por_limit=0.17
endif

if run_num=88
  shape_sep=1.9
  coef_fric=3
  por_limit=0.17
endif

if run_num=89
  shape_sep=2
  coef_fric=0.7
  por_limit=0.18
endif

if run_num=90
  shape_sep=2
  coef_fric=0.7
  por_limit=0.19
endif

if run_num=91
  shape_sep=2
  coef_fric=0.7
  por_limit=0.2
endif
if run_num=92
    shape_sep=2.1  
    coef_fric=.7  
    por_limit=.19
endif

if run_num=93
    shape_sep=2.1
    coef_fric=.6
    por_limit=.19
endif

    if run_num=94
        shape_sep=2.2
        coef_fric=.6
        por_limit=.19
    endif

if run_num=95
    shape_sep=2.1
    coef_fric=.6
    por_limit=.2
endif

if run_num=96
    shape_sep=2.2
    coef_fric=.5
    por_limit=.19
endif

if run_num=97
    shape_sep=2.2
    coef_fric=.55
    por_limit=.19
endif

if run_num=98
    shape_sep=2.1
    coef_fric=.6
    por_limit=.21
endif

if run_num=99
    shape_sep=2.1
    coef_fric=.6
    por_limit=.22
endif

if run_num=100
    shape_sep=2.1
    coef_fric=.6
    por_limit=.24
endif

if run_num=101
    shape_sep=2.1
    coef_fric=.65
    por_limit=.24
endif

if run_num=102
    shape_sep=2.1
    coef_fric=.65
    por_limit=.23
endif
if run_num=103
    shape_sep=2.1
    coef_fric=.7
    por_limit=.23
endif

if run_num=104
    coef_fric=.3
    ks_final=1e7
endif

if run_num=105
    coef_fric=.1
    ks_final=1e7
endif

if run_num=106
    coef_fric=3
    ks_final=1e7
endif

if run_num=107
    coef_fric=10
    ks_final=1e7
endif

if run_num=108
    coef_fric=.3
    ks_final=3e8
endif

if run_num=109
    coef_fric=.1
    ks_final=3e8
endif

if run_num=110
    coef_fric=3
    ks_final=3e8
endif

if run_num=111
    coef_fric=10
    ks_final=3e8
endif

if run_num=112
    coef_fric=.1
    ks_final=3e8
    shape_sep=1
endif

if run_num=113
    coef_fric=.3
    ks_final=3e8
    shape_sep=2
endif

if run_num=114
    coef_fric=1
    ks_final=3e8
    shape_sep=1.5
endif

if run_num=115
    coef_fric=3
    ks_final=3e8

shape_sep=2.5
endif

if run_num=116
  coef_fric=10
  ks_final=3e8
  shape_sep=1.5
endif

if run_num=117
  coef_fric=.1
  ks_final=1e7
  shape_sep=1
endif

if run_num=118
  coef_fric=.3
  ks_final=1e7
  shape_sep=2
endif

if run_num=119
  coef_fric=1
  ks_final=1e7
  shape_sep=1.5
endif

if run_num=120
  coef_fric=3
  ks_final=1e7
  shape_sep=2.5
endif

if run_num=121
  coef_fric=10
  ks_final=1e7
  shape_sep=1.5
endif

if run_num=122
  coef_fric=.1
  ks_final=1e8
  shape_sep=1
endif

if run_num=123
  coef_fric=.3
  ks_final=1e8
  shape_sep=1.5
endif

if run_num=124
  coef_fric=3
  ks_final=1e8
  shape_sep=2
endif

if run_num=125
  coef_fric=.1
  ks_final=1e8
  shape_sep=2.5
endif

if run_num=126
  coef_fric=3
  ks_final=1e8
  shape_sep=1
endif

if run_num=127
  coef_fric=10
  ks_final=1e8
  shape_sep=1.5
endif

if run_num=128
  coef_fric=10
  ks_final=1e8
  shape_sep=2
endif

if run_num=129
  coef_fric=3
  ks_final=1e8
  shape_sep=2.5
endif

if run_num=130
  coef_fric=1
  ks_final=1e7
  shape_sep=0
endif

if run_num=131
  coef_fric=.1
  kn_final=1e6
  ks_final=1e6
  shape_sep=0
endif

if run_num=132
  coef_fric=.3
  kn_final=1e6
  ks_final=1e6
  shape_sep=0
endif

if run_num=133
  coef_fric=1
  kn_final=1e6
  ks_final=1e6
  shape_sep=0
endif

if run_num=134
  coef_fric=3
  kn_final=1e6
  ks_final=1e6
  shape_sep=0
endif

if run_num=135 ;first attempt at calibration from the statistical model
  coef_fric=2
  kn_final=1e7
  ks_final=1e7
  shape_sep=1.77
  por_limit=.231
endif

if run_num=136 ;second attempt at calibration from the statistical model
  coef_fric=.7
  kn_final=1e7
  ks_final=1e7
  shape_sep=2.02
por_limit=.235
endif

if run_num=137 ;third attempt at calibration from the statistical model
coeff_fric=2
kn_final=1e8
ks_final=1e8
shape_sep=1.77
por_limit=.231
endif

if run_num=138 ;fourth attempt at calibration from the statistical model
coeff_fric=.7
kn_final=1e8
ks_final=1e8
shape_sep=2.02
por_limit=.235
endif

conf_press=75000*press_num
if press_num=0
  conf_press=30000
endif

if run_let='a'
  rand_seed=(10*run_num+press_num+.1)*10
endif

if run_let='b'
  rand_seed=(10*run_num+press_num+.2)*10
endif

if run_let='c'
  rand_seed=(10*run_num+press_num+.3)*10
endif

if run_let='d'
  rand_seed=(10*run_num+press_num+.4)*10
endif

if run_let='e'
  rand_seed=(10*run_num+press_num+.5)*10
endif

if run_let='f'
  rand_seed=(10*run_num+press_num+.6)*10
endif

kn_over_100=kn_final/100
ks_over_100=ks_final/100
end

;EOF case_conditions.dvr

iii. Make_d_shear.dvr

;set up window
set framewin pos 0 0 size .85 .85
set mainwin pos 0 .1 size 1 .9

call calc_gen_rad.dvr
set plot avi size 960 600

;CREATE BOX
wall id 1 nodes (xgen_min,0) (xgen_min,ygen_min)
wall id 1 kn kn_final ks ks_final fric coef_fric
wall id 2 nodes (xgen_min,ygen_min) (xgen_max,ygen_min)
wall id 2 kn kn_final ks ks_final fric coef_fric
wall id 3 nodes (xgen_max,ygen_min) (xgen_max,-.000001)
wall id 3 kn kn_final ks ks_final fric coef_fric
wall id 4 nodes (xgen_max,0) (room2move_right,0)
wall id 4 kn kn_final ks ks_final fric 0
wall id 5 nodes (xgen_max,0) (xgen_max,dilate_space)
wall id 5 kn kn_final ks ks_final fric coef_fric
wall id 6 nodes (xgen_max,ygen_max) (xgen_min,ygen_max)
wall id 6 kn kn_final ks ks_final fric coef_fric
wall id 7 nodes (xgen_min,dilate_space) (xgen_min,.000001)
wall id 7 kn kn_final ks ks_final fric_coef_fric
wall id 8 nodes (xgen_min,0) (room2move_left,0)
wall id 8 kn kn_final ks ks_final fric 0

call delstray.dvr

;CREATE SAND
set disk sys_thick
set max_balls num_to_gen
gen id 1,num_to_gen; x xgen_min,xgen_max y ygen_min,ygen_max rad r_gen_min,r_gen_max tries
100000
prop rad mul 2
prop den 2.65e3 kn kn_over_100 ks ks_over_100 fric 0

plot add wall black
plot add ball yellow outline off all on
plot set size p_lim_left p_lim_right p_lim_bottom p_lim_top

prop rad mul 2 kn mul 4 ks mul 4
solve average .001 maximum .001
prop rad mul 2 kn mul 4 ks mul 4
solve average .001 maximum .001
prop rad mul 2 kn mul 4 ks mul 4
solve average .001 maximum .001
prop kn mul 1.5625 ks mul 1.5625

def choose_clumps
  if shape_sep=0
    command
call ..\Tools\Sub_ball_nums.dat
  endcommand
  else
    command
call ..\Tools\Make_dyads.dat
  endcommand
  endif
end

choose_clumps

solve average .001 maximum .001

def y_pos
  y_pos=w_y(find_wall(20))
end

def stop_down
  if y_pos>y_stop
    stop_down=0
  else
    stop_down=1
endif
end

def stop_up
  if y_pos<y_stop
    stop_up=0
  else
    stop_up=1
  endif
end

call ..\FISH\servo.fis
call ..\FISH\fy_dt_old.fis

def variables
  k_p=1e0*USC
  k_i=2e5*USC
  k_d=1e-10*USC
  pressure=conf_press
end
variables

measure id 5 x 0 y 0 rad meas_rad

history id 1 nstep 10 press_y_act
history id 5 nstep 10 measure porosity id 5
history id 6 nstep 10 measure coord id 5
history id 9 nstep 10 wall_ypos
trace energy on

p create 1
p add hist 1
p create 5
p add hist 5
p create 6
p add hist 6
p create 9
p add hist 9

call ..\FISH\por_servo.fis
set wall_id 6
set target_por por_limit
call ..\FISH\equilibrium.fis

def variables
  k_p_por=10*sqrt(USC)
  k_i_por=100*sqrt(USC)
  k_d_por=1e-7*sqrt(USC)
  wall_add=find_wall(wall_id)
  seg_add=w_wlist(wall_add)
  m_add=find_meas(5)
  equil_limit=5e-6*USC
end
variables
set display fish w_yv
set fishcall 3 por_servo

save fname
solve average 0 maximum 0 fishhalt equilibrium
def por_servo
end
save fname2

; APPLY GRAVITY, CONFINING PRESSURE AND REACH EQUILIBRIUM
set grav 0,-9.81

prop fric coef_fric
set fishcall 3 servo
set equil_cntr 0
solve average 0 maximum 0 fishhalt equilibrium

call ..\FISH\zero_disp.fis
zero_disp ;ADDED 10/02/2009

plot current 0
plot sub 2
call vertlines.dat
save fname

iv. calc_gen_rad.dvr

;fname calc_gen_rad.dvr
call ..\FISH\calc_gen_rad.fis
def variables
  sys_thick=1
  xgen_min=-.025*USC
  xgen_max=.025*USC
  ygen_min=-.008*USC
  ygen_max=.008*USC
  room2move_left=1.5*xgen_min
  room2move_right=1.5*xgen_max
dilate_space=1.5*ygen_max
  p_lim_right=7*xgen_max/6
  p_lim_left=.2*xgen_max
  p_lim_top=ygen_max/3
  p_lim_bottom=ygen_min/3
  meas_rad=.0065*USC
  x_stop1=(xgen_max*2)/(5*4)
x_stop2=(xgen_max*2)/(5*2)
x_stop3=(xgen_max*2*3)/(5*4)
x_stop4=(xgen_max*2)/5
  x_stop_last=x_stop4
  shear_vel=xgen_max/(2.5*shear_time)
  min_max_factor=4 ;number of times larger the max radius is than the min radius for
uniformly graded specimen
target_pore=por_limit+.05
num_to_gen=10000
  num_to_gen_layer=num_to_gen/4
end
variables
calc_gen_rad
;EOF calc_gen_rad.dvr

v. Calc_gen_rad.fis

;fname calc_gen_rad.fis
;calculates radius limits for generate command
define calc_gen_rad
  pi_const=3.14159
  domain_area=(xgen_max-xgen_min)*(ygen_max-ygen_min)
  if min_max_factor=1
    r_gen_min=sqrt(domain_area*(1-target_pore)/(num_to_gen*pi_const))/16
  else

\[ r_{\text{gen\_min}} = \sqrt{3 \cdot \text{domain\_area} \cdot (1 - \text{target\_pore}) \cdot (\text{min\_max\_factor} - 1)} / (\pi \cdot \text{num\_to\_gen} \cdot (\text{min\_max\_factor}^3 - 1)) / 16; 16 \text{ is the factor of radius increase to fill the domain space after ball generation} \]

\[ r_{\text{gen\_max}} = \text{min\_max\_factor} \cdot r_{\text{gen\_min}} \]

\[ \text{EOF calc\_gen\_rad\_fis} \]

\section*{vi. Delstray.dvr}

; fname delstray.dvr

call ..\FISH\delstray.fis

def variables
    delstray\_freq=1000
    left\_lim\_add=find\_wall(1)
    right\_lim\_add=find\_wall(5)
    bottom\_lim\_add=find\_wall(2)
    top\_lim\_add=find\_wall(6)
end variables

set fishcall 3 delstray

; EOF delstray.dvr

\section*{vii. Delstray.fis}

; fname delstray.fis

def delstray

if cntr=delstray\_freq

    left\_limit=xgen\_min+w_x(left\_lim\_add)
    right\_limit=xgen\_max+w_x(right\_lim\_add)
    bottom\_limit=ygen\_min+w_y(bottom\_lim\_add)
    top\_limit=ygen\_max+w_y(top\_lim\_add)

    badd=ball\_head

    loop while badd # null
        next\_ball=b\_next(badd)
        if (b\_x(badd))<left\_limit
            ii=b\_delete(badd)
        else
            if (b\_x(badd))>right\_limit
                ii=b\_delete(badd)
            else
                if (b\_y(badd))<bottom\_limit
                    ii=b\_delete(badd)
                else
                    if (b\_y(badd))>top\_limit
                        ii=b\_delete(badd)
                endif
            endif
        endif
    endif
    badd=next\_ball
endloop
cntr=1
else
cntr=cntr+1
endif
end

;EOF delstray.fis

viii. Make_dyads.dat

clamp template make dyad 2 radii 1 1 position 0,0 shape_sep,0
clamp replace 1 dyad 1 range id 1,num_to_gen
clamp prop permanent

ix. Sub_ball_nums.dat

clamp template make ball_sub 1 radii 1 position 0,0
clamp replace 1 ball_sub 1 range id 1,num_to_gen

x. Servo.fis

;fname servo.fis
;moves wall in order to maintain constant force
;inputs: wall_id, pressure, k_p, k_i, k_d

def servo
  wall_add=find_wall(wall_id)
  seg_add=w_wlist(wall_add)
  x_length=abs(ws_length(seg_add)*ws_yun(seg_add))
  target_fy=pressure*x_length*sys_thick
  fy=w_yfob(wall_add)-target_fy
  press_y_act=w_yfob(wall_add)/(x_length*sys_thick)
  d_fy=fy-fy_old
  fy_dt_new=exp(-1000*abs(fy/target_fy))*(fy/target_fy)*tdel
  fy_dt=0.99*fy_dt+fy_dt_new
  p_term=k_p*(fy/target_fy)
  if p_term>USC*.02
    p_term=USC*.02
  else
    if p_term<-USC*.02
      p_term=-USC*.02
    endif
  endif
  i_term=k_i*f_y_dt
  d_term=k_d*d_fy/tdel*(fy/target_fy)^2
  if d_term>USC*.002
    d_term=USC*.002
  else
    if d_term<-USC*.002
      d_term=-USC*.002
    endif
  endif
  w_yv=(p_term+i_term+d_term)/(1000*exp(-30*abs(fy))+1)
  w_yvel(wall_add)=w_yv
  fy_old=fy

wall_ypos=w_y(wall_add)
end

\textbf{xii. \texttt{por_servo.fis}}

;fname \texttt{por_servo.fis}
;moves wall in order to achieve a given porosity
;inputs: wall_id, target_por

def por_servo
\[ x_{\text{length}} = \text{abs}(ws_{\text{length}}(seg_add) \times ws_{\text{yun}}(seg_add)) \]
\[ \text{por} = m_{\text{poros}}(m_{\text{add}}) - \text{target}_\text{por} \]
\[ d_{\text{por}} = \text{por} - \text{por}_{\text{old}} \]
if \text{por} > \text{por}_{\text{old}}
\[ \text{por}_{\text{dt}} = \text{por}_{\text{dt}} \times 0.1 \]
else
\[ \text{por}_{\text{dt}} = \exp(-\text{abs}(\text{por}/\text{target}_\text{por})) \times (\text{por}/\text{target}_\text{por}) \times \text{tdel} + \text{por}_{\text{dt}} \]
endif
\[ \text{p}_{\text{term}} = k_{\text{p}} \times \text{por}/\text{target}_\text{por} \]
\[ \text{i}_{\text{term}} = k_{\text{i}} \times \text{por}_{\text{dt}} \]
\[ \text{d}_{\text{term}} = k_{\text{d}} \times \text{por}_{\text{dt}}/\text{tdel} \times (\text{por}/\text{target}_\text{por})^2 \]
\[ w_{\text{yv}} = \text{p}_{\text{term}} + \text{i}_{\text{term}} + \text{d}_{\text{term}} \]
\[ w_{\text{yvel}}(\text{wall}_{\text{add}}) = -w_{\text{yv}} \]
\[ \text{por}_{\text{old}} = \text{por} \]
wall_ypos=w_y(wall_add)
end
xiii. Equilibrium.fis

;fname equilibrium.fis
;uses average unbalanced force to decide when a simulation
;has reached equilibrium
;required input: equil_limit (equil. value for average FOB)

define equilibrium
if av_unbal<equil_limit
    equil_cntr=equil_cntr+1
    if equil_cntr>1000
        equilibrium=1
    else
        equilibrium=0
    endif
end

;EOF equilibrium.fis

xiv. Zero_disp.fis

define zero_disp
badd=ball_head
loop while badd # null
    b_rot(badd)=0
    b_xdisp(badd)=0
    b_ydisp(badd)=0
    badd=b_next(badd)
endloop
end

xv. vertlines.dat

set echo off
range name range6 x -0.025125 -0.024875 y -0.008 0.008
range name range8 x -0.022625 -0.022375 y -0.008 0.008
range name range10 x -0.020125 -0.019875 y -0.008 0.008
range name range12 x -0.017625 -0.017375 y -0.008 0.008
range name range14 x -0.015125 -0.014875 y -0.008 0.008
range name range16 x -0.012625 -0.012375 y -0.008 0.008
range name range18 x -0.010125 -0.009875 y -0.008 0.008
range name range20 x -0.007625 -0.007375 y -0.008 0.008
range name range22 x -0.005125 -0.004875 y -0.008 0.008
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<th>Y-Range</th>
<th>Width</th>
<th>Height</th>
<th>X-Position</th>
<th>Y-Position</th>
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<td>0.020125</td>
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<td>0.025</td>
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<td>-0.008</td>
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<tr>
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<td>-0.025025</td>
<td>0.025</td>
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<td>-0.008</td>
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<td>range54</td>
<td>-0.025025</td>
<td>0.025</td>
<td>y</td>
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<td>0.025</td>
<td>y</td>
<td>-0.008</td>
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<td>0.025</td>
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<td>-0.008</td>
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<td>range60</td>
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<td>0.025</td>
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range name range142 x 0.020125 0.022375 y -0.005375
  -0.003125
  group blue_group range range142
range name range144 x 0.022625 0.024875 y -0.005375
  -0.003125
  group green_group range range144
range name range146 x 0.025125 0.027375 y -0.005375
  -0.003125
  group red_group range range146
range name range148 x -0.024875 -0.022625 y -0.002875
  -0.000625
  group red_group range range148
range name range150 x -0.022375 -0.020125 y -0.002875
  -0.000625
  group yellow_group range range150
range name range152 x -0.019875 -0.017625 y -0.002875
  -0.000625
  group blue_group range range152
range name range154 x -0.017375 -0.015125 y -0.002875
  -0.000625
  group green_group range range154
range name range156 x -0.014875 -0.012625 y -0.002875
  -0.000625
  group red_group range range156
range name range158 x -0.012375 -0.010125 y -0.002875
  -0.000625
  group yellow_group range range158
range name range160 x -0.009875 -0.007625 y -0.002875
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  group blue_group range range160
range name range162 x -0.007375 -0.005125 y -0.002875
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range name range166 x -0.002375 -0.000125 y -0.002875
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range name range170 x 0.002625 0.004875 y -0.002875
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range name range172 x 0.005125 0.007375 y -0.002875
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<td>0.022625</td>
<td>0.024875</td>
<td>0.00212</td>
<td>0.004375</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>range270</td>
<td></td>
<td>0.025125</td>
<td>0.027375</td>
<td>0.00212</td>
<td>0.004375</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>range272</td>
<td></td>
<td>0.027625</td>
<td>0.029875</td>
<td>0.00212</td>
<td>0.004375</td>
<td></td>
<td></td>
</tr>
<tr>
<td>range name</td>
<td>x</td>
<td>y</td>
<td>group</td>
<td>range name</td>
<td>x</td>
<td>y</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-------------</td>
<td>-----------</td>
<td>-----------</td>
<td>-------</td>
<td>-------------</td>
<td>-----------</td>
<td>-----------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>range274</td>
<td>-0.024875</td>
<td>-0.022625</td>
<td>red</td>
<td>range274</td>
<td>-0.022375</td>
<td>-0.020125</td>
<td></td>
<td></td>
</tr>
<tr>
<td>range274</td>
<td>-0.022375</td>
<td>-0.020125</td>
<td>yellow</td>
<td>range276</td>
<td>-0.019875</td>
<td>-0.017625</td>
<td></td>
<td></td>
</tr>
<tr>
<td>range280</td>
<td>-0.017375</td>
<td>-0.015125</td>
<td>blue</td>
<td>range278</td>
<td>-0.014875</td>
<td>-0.012625</td>
<td></td>
<td></td>
</tr>
<tr>
<td>range282</td>
<td>-0.012375</td>
<td>-0.010125</td>
<td>red</td>
<td>range284</td>
<td>-0.009875</td>
<td>-0.007625</td>
<td></td>
<td></td>
</tr>
<tr>
<td>range286</td>
<td>-0.007375</td>
<td>-0.005125</td>
<td>blue</td>
<td>range288</td>
<td>-0.005125</td>
<td>-0.002625</td>
<td></td>
<td></td>
</tr>
<tr>
<td>range290</td>
<td>-0.004875</td>
<td>-0.002625</td>
<td>red</td>
<td>range292</td>
<td>-0.002375</td>
<td>-0.000125</td>
<td></td>
<td></td>
</tr>
<tr>
<td>range294</td>
<td>0.000125</td>
<td>0.002375</td>
<td>blue</td>
<td>range294</td>
<td>0.002625</td>
<td>0.004875</td>
<td></td>
<td></td>
</tr>
<tr>
<td>range296</td>
<td>0.005125</td>
<td>0.007375</td>
<td>green</td>
<td>range298</td>
<td>0.007625</td>
<td>0.009875</td>
<td></td>
<td></td>
</tr>
<tr>
<td>range300</td>
<td>0.007625</td>
<td>0.009875</td>
<td>red</td>
<td>range302</td>
<td>0.010125</td>
<td>0.012375</td>
<td></td>
<td></td>
</tr>
<tr>
<td>range304</td>
<td>0.012625</td>
<td>0.014875</td>
<td>blue</td>
<td>range304</td>
<td>0.015125</td>
<td>0.017375</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
range name range340  x  0.005125  0.007375  y  0.007125
0.009375
group red_group range range340

range name range342  x  0.007625  0.009875  y  0.007125
0.009375
group yellow_group range range342

range name range344  x  0.010125  0.012375  y  0.007125
0.009375
group blue_group range range344

range name range346  x  0.012625  0.014875  y  0.007125
0.009375
group green_group range range346

range name range348  x  0.015125  0.017375  y  0.007125
0.009375
group red_group range range348

range name range350  x  0.017625  0.019875  y  0.007125
0.009375
group yellow_group range range350

range name range352  x  0.020125  0.022375  y  0.007125
0.009375
group blue_group range range352

range name range354  x  0.022625  0.024875  y  0.007125
0.009375
group green_group range range354

range name range356  x  0.025125  0.027375  y  0.007125
0.009375
group red_group range range356

plot add ball red range group red_group outline off all on
plot add ball yellow range group yellow_group outline off all on
plot add ball blue range group blue_group outline off all on
plot add ball green range group green_group outline off all on
plot add ball black range group black_group outline off all on

set echo on

xvi.  direct_shear.dvr

set logfile fname
set log on

def real_stress
  tot_force=w_xfob(find_wall(5))+w_xfob(find_wall(6))+w_xfob(find_wall(7))
  x_pos=w_x(find_wall(6))
  real_stress=-tot_force/(sys_thick*(xgen_max-xgen_min-x_pos))
  avi_name=fname+'.avi'
end

real_stress

del hist

hist id 6 nstep 100 x_pos
hist id 1 nstep 100 press_y_act
p cur 1
p clear
p add hist 1 vs 6
hist id 5 nstep 100 real_stress
p cur 5
p clear
p add hist 5 vs 6
hist id 8 nstep 100 measure por id 5
p cur 6
p clear
p add hist 8 vs 6
hist id 9 nstep 100 wall_ypos
p cur 9
p clear
p add hist 9 vs 6

def variables
  p_lim_left=1.5*xgen_min
  p_lim_right=xgen_min/3
  p_lim_top=ygen_max/2
  p_lim_bottom=ygen_min/2
  mov_step_freq=.005/tdel ;(This value will create about 20 seconds of video per second of simulated time at 10 frames/sec)
end

variables

p cur 0
plot set window pos 0 0 size 1 .8
plot set caption size 20
plot set size p_lim_left p_lim_right p_lim_bottom p_lim_top
p add hist 5 vs 6 pos 0 0 .45 1
p move 7 1
p add meas white

wall id 5 xv shear_vel
wall id 6 xv shear_vel
wall id 7 xv shear_vel
wall id 8 xv shear_vel

def stop
  if x_pos<x_stop
    stop=0
  else
    stop=1
  endif
end

set display fish x_pos

set plot avi size 1280 800
movie step mov_step_freq 0 file avi_name
movie avi_open file avi_name

print shear_vel
set x_stop x_stop1
solve average 0 maximum 0 fishhalt stop
save fname2

set x_stop x_stop2
solve average 0 maximum 0 fishhalt stop
save fname2

set x_stop x_stop3
solve average 0 maximum 0 fishhalt stop
save fname2

set x_stop x_stop4
solve average 0 maximum 0 fishhalt stop

history write 5 vs 6 skip 100 file fname
movie avi_close file avi_name

plot current 5
plot set caption off
plot set background white
set plot bmp size 600 600
def variables
  bname=fname+'.bmp'
end
variables
set output bname
plot hard
save fname2
set log off

b. MGR Wheel/Soil Codes

Note that by changing the two variables (run_num and run_let) in the main driver file for the MGR Rigid wheel simulation, the parameters of the simulation are automatically selected.

i. MGR_Rigid_03a.dvr

;filename MGR_Rigid_03a.dvr

new

def variables
  run_num=03
  run_let='a'
  fname='MGR_Rigid_0'+string(run_num)+run_let
  fname2=fname+'_final'
  avi_name1=fname+'_1.avi'
  avi_name2=fname+'_2.avi'
  avi_name3=fname+'_3.avi'
end
variables
set logfile fname
set log on
call case_conditions.dvr
case_conditions
set rand rand_seed
call calc_gen_rad.dvr
call ..\FISH\ck_pt_solve.fis
call make_MGR.dvr
call MGR_wheel.dvr
print fname
set log off
;EOF 'fname'+.dvr
ii. Case_conditions.dvr

;fname case_conditions.dvr
;selects parameters based on run number and pressure number
;run letter -> random specimen id

def case_conditions

    if run_num=01 ;round, small diameter
        vert_mass=140.2*4.44822/9.81
        Ig=59.55*.009415 ;*(.0254*4.448)/12 converts slug*in^2 to N*m*s^2
        wheel_avg_rad=.2606
        make_wheel_fname='round_small.dat'
        num_wheel_walls=1
    endif

    if run_num=02 ;64 square grousers
        vert_mass=145.4*4.44822/9.81
        Ig=77.9*.009415
        wheel_avg_rad=2.811 ;(.2811*2.548*64+.2606*(360-2.548*64))/360 Note: expression for average radius weighted by subtended angle was replaced by a fixed value because of presence of the same error in the MGR lab experiments.
        make_wheel_fname='64_square.dat'
        num_wheel_walls=2
    endif

    if run_num=03 ;64 sharp grousers
        vert_mass=142.8*4.44822/9.81
        Ig=64.1*.009415
        wheel_avg_rad=2.811 ;((.2811*.3333+.2606*.6666)*2.548*64+.2606*(360-2.548*64))/360
        make_wheel_fname='64_sharp.dat'
        num_wheel_walls=2
    endif

    if run_num=04 ;32 sharp grousers
        vert_mass=141.5*4.44822/9.81
        Ig=61.8*.009415
        wheel_avg_rad=2.811 ;((.2811*.3333+.2606*.6666)*2.548*32+.2606*(360-2.548*32))/360
        make_wheel_fname='32_sharp.dat'
        num_wheel_walls=2
    endif

    if run_num=05 ;16 sharp grousers
        vert_mass=140.8*4.44822/9.81
        Ig=61.8*.009415
        wheel_avg_rad=2.811 ;((.2811*.3333+.2606*.6666)*2.548*16+.2606*(360-2.548*16))/360
        make_wheel_fname='16_sharp.dat'
        num_wheel_walls=2
    endif

    if run_num=06 ;round, large diameter
        vert_mass=154*4.44822/9.81
        Ig=102.7*.009415
        wheel_avg_rad=.2811
        make_wheel_fname='round_large.dat'
        num_wheel_walls=1
    endif

    if run_let='a'
        rand_seed=(10*run_num+1)
    endif

    if run_let='b'

165
rand_seed=(10*run_num+2)
endif
if run_let='c'
  rand_seed=(10*run_num+3)
endif
if run_let='d'
  rand_seed=(10*run_num+4)
endif
if run_let='e'
  rand_seed=(10*run_num+5)
endif
if run_let='f'
  rand_seed=(10*run_num+6)
endif
end
;EOF case_conditions.dvr

iii. Calc_gen_rad.dvr

;fnamecalc_gen_rad.dvr
call ..\FISH\calc_gen_rad.fis
def variables
;miscellaneous variables
  ck_pt_clock=240 ;minutes. Used by the ck_pt_solv e function; specifies computer runtime
  on a given solve command before a checkpoint is saved
;soil box properties
  sys_thick=6.125*.0254
  xgen_min=-.5  
  xgen_max=2.5
  ygen_min=-.537
  ygen_max=+.3
  dilate_space=.05
  wall_top=ygen_max+dilate_space
  p_lim_right=2.6
  p_lim_left=.6
  p_lim_top=.3
  p_lim_bottom=.45
  meas_rad=(0.4*(ygen_max-ygen_min))
  meas_y=(ygen_min+ygen_max)/2-0.095*(ygen_max-ygen_min)
  meas_spacing=(xgen_max-xgen_min-4*meas_rad)/4
  meas1_x=xgen_min+2*meas_rad
  meas2_x=meas1_x+meas_spacing
  meas3_x=meas2_x+meas_spacing
  meas4_x=meas3_x+meas_spacing
  meas5_x=meas4_x+meas_spacing
  wall_fric=10
;soil properties
  coef_fric=.7
  shape_sep=2.02
kn_final=1e7
ks_final=1e7
por_limit=.235
kn_over_256=kn_final/256
ks_over_256=ks_final/256

;wheel properties

horiz_mass=2728
wheel_fric=10
wheel_alpha=-(0.3*1000)/(3600*wheel_avg_rad)
w_b_mom_max=6.66 \ N*m

;particle size calculation

min_max_factor=4 ;number of times larger the max radius is than the min radius for
uniformly graded specimen
target_pore=por_limit+.05
num_to_gen=25000
max_balls_number=1.2*num_to_gen
end

variables

calc_gen_rad

;EOF calc_gen_rad.dvr

iv. Calc_gen_rad.fis

;fname calc_gen_rad.fis
;calculates radius limits for generate command
define calc_gen_rad
pi_const=3.14159
domain_area=(xgen_max-xgen_min)*(ygen_max-ygen_min)
if min_max_factor=1
  r_gen_min=sqrt(domain_area*(1-target_pore)/(num_to_gen*pi_const))/16
else
  r_gen_min=sqrt(3*domain_area*(1-target_pore)*(min_max_factor-1)/(pi_const*num_to_gen*(min_max_factor^3-1)))/16 ;16 is the factor of radius increase to
fill the domain space after ball generation
endif
r_gen_max=min_max_factor*r_gen_min
end

;EOF calc_gen_rad.fis

v. Check_pt_solve.fis

;performs solve command repeatedly with periodic breaks for checkpoint saving
;the 'comment' variable is a string describing the current phase. It is displayed during
cycling to allow easy recognition of simulation progress
def ck_pt_solve

ck_pt_run=ck_pt_run+1 ;tracks which instance of solve command is being manipulated
ck_pt_complete=0 ;tracks whether crash occurred during or between solves
equil_cntr=0
done=0

loop while done=0
  command
    print comment
solve ave ck_pt_ave max ck_pt_max time ck_pt_time clock ck_pt_clock fish equilibrium
save fname2
end_command

done=1 ;default
if av_unbal/av_cforce<ck_pt_ave
else
  if max_unbal/max_cforce<ck_pt_max
  else
    if time>ck_pt_time
    else
      if equilibrium=1
      else
        done=0 ;because termination of SOLVE was due to timeout for checkpointing
      end_if
    end_if
  end_if
else
  end_if
end_if
end_loop

ck_pt_complete=1
end
ck_pt_run=0

vi. Make_MGR.dvr

;set up window
set framewin pos 0 0 size .85 .85
set mainwin pos 0 .1 size 1 .9

;CREATE BOX
wall id 101 nodes (xgen_min,wall_top) (xgen_min,ygen_min)
wall id 101 kn kn_final ks ks_final fric wall_fric
wall id 102 nodes (xgen_min,ygen_min) (xgen_max,ygen_min))
wall id 102 kn kn_final ks ks_final fric wall_fric
wall id 103 nodes (xgen_max,ygen_min) (xgen_max,wall_top)
wall id 103 kn kn_final ks ks_final fric wall_fric
wall id 104 nodes (xgen_max,ygen_max) (xgen_min,ygen_max)
wall id 104 kn kn_final ks ks_final fric wall_fric

call delstray.dvr

;CREATE SAND
set disk sys_thick
set max_balls max_balls_number
gen id 1,num_to_gen x xgen_min,xgen_max y ygen_min,ygen_max rad r_gen_min,r_gen_max tries 1000000
prop rad mul 2
prop den 2.65e3 kn kn_over_256 ks ks_over_256 fric 0
plot add wall black
plot add ball yellow outline off all on
plot set size p_lim_left p_lim_right p_lim_bottom p_lim_top
cycle 1
def variables
  mov_step_freq=.1/tdel ;this value produces about 1 second of video per second of simulation (actual speed)
  comment='description of current phase of computation'
end variables
plot set background white
plot set caption off
set plot avi size 1280 800
movie step mov_step_freq 0 file avi_name1
movie avi_open file avi_name1

call ..\FISH\equilibrium.fis

def ck_pt_vars
  ck_pt_ave=.01
  ck_pt_max=.01
  ck_pt_time=1e6 ;seconds
  equil_limit=1e-5
end
ck_pt_vars

prop rad mul 2 kn mul 4 ks mul 4
set comment 'ck_pt_run=1'
ck_pt_solve  ;ck_pt_run=1
  ;ck_pt_solve function executes checkpoint
  saving
set equilibrium 0
prop rad mul 2 kn mul 4 ks mul 4
set comment 'ck_pt_run=2'
ck_pt_solve  ;EXPAND BALLS 2        ;ck_pt_run=2
set equilibrium 0
prop rad mul 2 kn mul 4 ks mul 4
set comment 'ck_pt_run=3'
ck_pt_solve  ;EXPAND BALLS 3        ;ck_pt_run=3
set equilibrium 0
prop kn mul 4 ks mul 4

def choose_clumps
  if shape_sep=0
    command
call ..\Tools\Sub_ball_nums.dat
  endcommand
else
  command
call ..\Tools\Make_dyads.dat
  endcommand
endif
choose_clumps

def ck_pt_vars
  ck_pt_ave=.01
  ck_pt_max=.01
  ck_pt_time=1e6 ;seconds
  equil_limit=1e-5
end
ck_pt_vars

set comment 'SETTLE CLUMPS'
ck_pt_solve  ;SETTLE CLUMPS            ;ck_pt_run=4
set equilibrium 0

measure id 1 x meas1_x y meas_y rad meas_rad
measure id 2 x meas2_x y meas_y rad meas_rad
measure id 3 x meas3_x y meas_y rad meas_rad
measure id 4 x meas4_x y meas_y rad meas_rad
measure id 5 x meas5_x y meas_y rad meas_rad

define find_meas_add
  m_add1=find_meas(1)
m_add2=find_meas(2)
m_add3=find_meas(3)
m_add4=find_meas(4)
m_add5=find_meas(5)
end
find_meas_add

define avg_por

avg_por=(m_poros(m_add1)+m_poros(m_add2)+m_poros(m_add3)+m_poros(m_add4)+m_poros(m_add5))\n/5
end

call ..\FISH\por_servo_MGR.fis
set target_por por_limit
def variables
  k_p_por=1
  k_i_por=1
  k_d_por=1e-7
  wall_add=find_wall(104)
end variables
set display fish w_yv
set fishcall 3 por_servo

history id 2 nstep 10 avg_por
history id 3 nstep 10 w_yv

p create 1
p add wall black
p add ball yellow outline off all on
plot set size 0 .3 -.45 -.15

p create 2
p add hist 2
p create 3
p add hist 3

p cur 0
plot set background gray .9

def ck_pt_vars
  ck_pt_ave=.001
  ck_pt_max=.001
  ck_pt_time=1e6 ;seconds
  equil_limit=1e-3
end
ck_pt_vars

set comment 'ACHIEVE POROSITY'
ck_pt_solve ;ACHIEVE POROSITY ;ck_pt_run=5
set equilibrium 0

set fishcall 3 remove por_servo

plot set background white

;APPLY GRAVITY, remove lid AND REACH EQUILIBRIUM
set grav 0,-9.81

prop fric coef_fric

wall id 104 yv .01

def ck_pt_vars
  ck_pt_ave=.01
  ck_pt_max=.01
  ck_pt_time=1e6 ;seconds
  equil_limit=1e-3
end
ck_pt_vars
set comment 'REMOVE CONFINING WALL AND SETTLE'
ck_pt_solve ;REMOVE CONFINING WALL AND SETTLE ;ck_pt_run=6
set equilibrium 0

movie avi_close file avi_name1
delete wall 104

call ..\FISH\zero_disp.fis
zero Disp ;ADDED 10/02/2009

plot current 0
plot sub 2
call vertlines.dat
p cur 1
p sub 2
plot add ball red range group red_group outline off all on
plot add ball yellow range group yellow_group outline off all on
plot add ball blue range group blue_group outline off all on
plot add ball green range group green_group outline off all on
plot add ball black range group black_group outline off all on
save fname

set time 0

vii. Delstray.dvr

;fname delstray.dvr
call ..\FISH\delstray_MGR.fis
def variables
delstray_freq=1000
left_lim_add=find_wall(101)
right_lim_add=find_wall(103)
bottom_lim_add=find_wall(102)
end
variables
set fishcall 3 delstray
;EOF delstray.dvr

viii. Delstray_MGR.fis

;fname delstray_MGR.fis
def delstray
if cntr=delstray_freq
left_limit=xgen_min+w_x(left_lim_add)
right_limit=xgen_max+w_x(right_lim_add)
bottom_limit=ygen_min+w_y(bottom_lim_add)
top_limit=ygen_max+2*dilate_space
badd=ball_head
loop while badd # null
next_ball=b_next(badd)
if (b_x(badd))<left_limit
li=b_delete(badd)
else
if (b_x(badd))>right_limit
   ii=b_delete(badd)
else
   if (b_y(badd))<bottom_limit
      ii=b_delete(badd)
   else
      if (b_y(badd))>top_limit
         ii=b_delete(badd)
      endif
   endif
endif
endif
endif
badd=next_ball
endloop
cntr=1
else
cntr=cntr+1
endif
end

;EOF delstray_MGR.fis

ix. Equilibrium.fis

;fname equilibrium.fis
;uses average unbalanced force to decide when a simulation
;has reached equilibrium
;required input: equil_limit (equil. value for average FOB)

define equilibrium
  if av_unbal<equil_limit
    equil_cntr=equil_cntr+1
  if equil_cntr>1000
    equilibrium=1
  else
    equilibrium=0
  endif
endif
end

;EOF equilibrium.fis

x. Por_servo_MGR.fis

;fname por_servo.fis
;moves wall in order to achieve a given porosity
;inputs: wall_id, target_por

def por_servo
  por=avg_por-target_por
  d_por=por-por_old
  if por*por_old<0
    por_dt=por_dt*.1
  else
    por_dt=exp(-abs(por/target_por))*(por/target_por)*tdel+por_dt
  endif
  p_term=k_p_por*por/target_por
  i_term=k_i_por*por_dt
  d_term=k_d_por*d_por/tdel*(por/target_por)^2
  w_yv=p_term+i_term+d_term
  w_yvel(wall_add)=-w_yv
por_old=por
wall_ypos=w_y(wall_add)
end

xi. zero_disp.fis

define zero_disp
badd=ball_head
loop while badd # null
b_rot(badd)=0
b_xdisp(badd)=0
b_ydisp(badd)=0
badd=b_next(badd)
endloop
end

xii. vertlines.dat

range name range6 x -0.505 -0.495 y -0.45 -0.25
range name range8 x -0.405 -0.395 y -0.45 -0.25
range name range10 x -0.305 -0.295 y -0.45 -0.25
range name range12 x -0.205 -0.195 y -0.45 -0.25
range name range14 x -0.105 -0.095 y -0.45 -0.25
range name range16 x -0.005 0.005 y -0.45 -0.25
range name range18 x 0.095 0.105 y -0.45 -0.25
range name range20 x 0.195 0.205 y -0.45 -0.25
range name range22 x 0.295 0.305 y -0.45 -0.25
range name range24 x 0.395 0.405 y -0.45 -0.25
range name range26 x 0.495 0.505 y -0.45 -0.25
range name range28 x 0.595 0.605 y -0.45 -0.25
range name range30 x 0.695 0.705 y -0.45 -0.25
range name range32 x 0.795 0.805 y -0.45 -0.25
range name range34 x 0.895 0.905 y -0.45 -0.25
range name range36 x 0.995 1.005 y -0.45 -0.25
range name range38 x 1.095 1.105 y -0.45 -0.25
range name range40 x 1.195 1.205 y -0.45 -0.25
range name range42 x 1.295 1.305 y -0.45 -0.25
range name range44 x 1.395 1.405 y -0.45 -0.25
range name range46 x 1.495 1.505 y -0.45 -0.25
range name range48 x 1.595 1.605 y -0.45 -0.25
range name range50 x 1.695 1.705 y -0.45 -0.25
;fname MGR_wheel.dvr

delete hist
plot destroy 3

def variables
    mov_step_freq=.1/tdel ;this value produces about 1 second of video per second of simulation (actual speed)
end variables

plot current 0
plot set background gray .9
plot set caption off
set plot avi size 1280 800
movie step mov_step_freq 0 file avi_name2
movie avi_open file avi_name2

plot current 1
plot set background gray .9
plot set caption off
movie step mov_step_freq 1 file avi_name3
movie avi_open file avi_name3

call make_wheel_fname
call wheel_translation.dvr
set display fish wall\_yf

set wheel_lower\_rate -100
set coarse\_stop\_fraction 0
wheel\_coarse\_lower ;FIRST TIME, 100 M/S
set ck\_pt\_run 7
solve average 0 maximum 0 fish wheel\_coarse\_stop ;ck\_pt\_run=7
save fname2

set wheel_lower\_rate -.01
set coarse\_stop\_fraction .8
set wheel\_coarse\_stop 0
wheel\_coarse\_lower ;SECOND TIME, 0.01 M/S
set ck\_pt\_run 8
solve average 0 maximum 0 fish wheel\_coarse\_stop ;ck\_pt\_run=8
save fname2

set fishcall 3 wheel\_Newton\_trans

def ck\_pt\_vars
    ck\_pt\_ave=.01
    ck\_pt\_max=.01
    ck\_pt\_time=1e6 ;seconds
    equil\_limit=1e-3
end ck\_pt\_vars
set comment 'WHEEL SETTLING'
call ck\_pt\_solve ;WHEEL SETTLING ;ck\_pt\_run=9
set equilibrium 0

p cur 0
plot set background white
p cur 1
plot set background white
call wheel_rotation.dvr

set fishcall 3 wheel_a_acc

define variables
    a_start_time=time
    cv_start_time=a_start_time+3.333
    cv_stop_time=cv_start_time+8
end

variables

def rot_time
    rot_time=time-a_start_time
end

hist id 1 nstep 100 rot_time
hist id 2 nstep 100 wheel_kph
hist id 3 nstep 100 MGR_kph

set display fish MGR_kph

p cur 2
p sub 1
p add hist -2 vs 1 ymax 1.2
p add hist 3 vs 1 ymax 1.2

def ck_pt_vars
    ck_pt_ave=0
    ck_pt_max=0
    ck_pt_time=cv_start_time ;seconds
    equil_limit=0
end

ck_pt_vars

print cv_start_time ;STEP ENDS AT THIS TIME

def variables
    comment='CONSTANT ACCELERATION (ends at time '+string(cv_start_time)+')'
end

variables

ck_pt_solve ;CONSTANT ACCELERATION ;ck_pt_run=10

movie avi_close file avi_name3

set fishcall 3 remove wheel_a_acc

p cur 0
plot set background gray .9
p cur 1
plot set background gray .9

def wheel_speed
    if MGR_kph>wheel_speed_limit
        wheel_speed=1
    else
        wheel_speed=0
    endif
end

call ..\FISH\ck_pt_solve2.fis

def ck_pt_vars
    ck_pt_ave=0
    ck_pt_max=0
    ck_pt_time=1e6 ;seconds
    wheel_speed_limit=0.9
end
ck_pt_vars

def variables
    comment='CONSTANT VELOCITY (ends when MGR_kph = '+string(wheel_speed_limit)+')'
end
variables
ck_pt_solve2 ;CONSTANT VELOCITY ;ck_pt_run=11

def ck_pt_vars
    cv_stop_time=time+2
    ck_pt_ave=0
    ck_pt_max=0
    ck_pt_time=cv_stop_time ;seconds
    equil_limit=0
end
ck_pt_vars

print cv_stop_time ;STEP ENDS AT THIS TIME

def variables
    comment='CONSTANT VELOCITY (ends at time '+string(cv_stop_time)+')'
end
variables
ck_pt_solve ;CONSTANT VELOCITY ;ck_pt_run=12

p cur 0
plot set background white
p cur 1
plot set background white

set fishcall 3 wheel_Newton_rot

def ck_pt_vars
    ck_pt_ave=.0001
    ck_pt_max=.0001
    ck_pt_time=1e6 ;seconds
    equil_limit=1e-3
end
ck_pt_vars

set comment 'DECELERATION TO REST (ENDS AFTER SETTLING)'
ck_pt_solve ;DECELERATION TO REST (ENDS AFTER SETTLING) ;ck_pt_run=13

movie avi_close file avi_name2

xiv.  64_sharp.dat (called by variable “make_wheel_fname”)
<table>
<thead>
<tr>
<th>wall id 1</th>
<th>nodes</th>
<th>x1</th>
<th>y1</th>
<th>z1</th>
<th>x2</th>
<th>y2</th>
<th>z2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>wall id 1</td>
<td>-0.178327952</td>
<td>-0.217293238</td>
<td>0.144387057</td>
<td>-0.19468341</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>wall id 1</td>
<td>-0.156170793</td>
<td>-0.233726108</td>
<td>0.124609483</td>
<td>-0.20789363</td>
<td></td>
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</tr>
<tr>
<td></td>
<td>wall id 1</td>
<td>-0.132509623</td>
<td>-0.247908067</td>
<td>0.103631851</td>
<td>-0.21911114</td>
<td></td>
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</tr>
<tr>
<td></td>
<td>wall id 1</td>
<td>-0.107572313</td>
<td>-0.259702537</td>
<td>0.081656188</td>
<td>-0.228213758</td>
<td></td>
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<tr>
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<td>-0.081599023</td>
<td>-0.268995928</td>
<td>0.058894131</td>
<td>-0.235118552</td>
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<tr>
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<td>-0.275698742</td>
<td>0.035564892</td>
<td>-0.239759027</td>
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<tr>
<td></td>
<td>wall id 1</td>
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<td>-0.279746427</td>
<td>0.011893143</td>
<td>-0.24209049</td>
<td></td>
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<td>-0.17959355</td>
<td>-0.162774105</td>
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<tr>
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<td>-0.198767716</td>
<td>-0.162774105</td>
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<tr>
<td></td>
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<td>-0.217293238</td>
<td>-0.17959355</td>
<td>-0.162774105</td>
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<td>-0.162774105</td>
<td>-0.17959355</td>
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</tr>
</tbody>
</table>
wall id 1 nodes -0.156170793 0.233726108 -0.124609483 0.207898363
wall id 1 nodes -0.132509623 0.247908067 -0.103631851 0.21911114
wall id 1 nodes -0.107572313 0.259702537 -0.081656188 0.228213758
wall id 1 nodes -0.081599023 0.268995928 -0.058894131 0.235118552
wall id 1 nodes -0.05483989 0.275698742 -0.035564892 0.239759027
wall id 1 nodes -0.027552618 0.279746427 -0.011893143 0.24209049
wall id 1 nodes -5.16584E-17 0.2811 0.011893143 0.24209049
wall id 1 nodes 0.027552618 0.279746427 0.035564892 0.239759027
wall id 1 nodes 0.05483989 0.275698742 0.058894131 0.235118552
wall id 1 nodes 0.081599023 0.268995928 0.081656188 0.228213758
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wall id 1 nodes 0.156170793 0.233726108 0.144387057 0.19468341
wall id 1 nodes 0.178327952 0.217293238 0.162774105 0.17959355
wall id 1 nodes 0.198767716 0.198767716 0.17959355 0.162774105
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wall id 1 nodes 0.275698742 0.05483989 0.239759027 0.035564892
wall id 1 nodes 0.279746427 0.027552618 0.24209049 0.011893143 0.2811

xv. *Wheel_translation.dvr*

;fname wheel_translation.dvr

define find_wheel_add
array wheel_add(num_wheel_walls)
loop nn (1,num_wheel_walls-1)
    wheel_add(nn)=find_wall(nn)
end_loop
wheel_add(num_wheel_walls)=find_wall(100)
end

find_wheel_add

define wheel_coarse_lower
loop nn (1,num_wheel_walls)
    w_yvel(wheel_add(nn))=wheel_lower_rate
end_loop
define wheel_coarse_stop
  wall_yf=0
  loop nn (1,num_wheel_walls)
    wall_yf=wall_yf+w_yfob(wheel_add(nn))
  end_loop
  if wall_yf>coarse_stop_fraction*9.81*vert_mass
    wheel_coarse_stop=1
  else
    wheel_coarse_stop=0
  endif
end

define wheel_Newton_trans
  wall_xf=0
  wall_yf=0
  loop nn (1,num_wheel_walls)
    wall_xf=wall_xf+w_xfob(wheel_add(nn))
    wall_yf=wall_yf+w_yfob(wheel_add(nn))
  end_loop
  wheel_xa=wall_xf/horiz_mass
  wheel_ya=wall_yf/vert_mass-9.81
  wheel_xv=wheel_xv+wheel_xa*tdel
  MGR_kph=wheel_xv*3.6
  wheel_ya=wall_yf/vert_mass-9.81
  wheel_yv=wheel_yv+wheel_ya*tdel
  loop nn (1,num_wheel_walls)
    w_xvel(wheel_add(nn))=wheel_xv
    w_yvel(wheel_add(nn))=wheel_yv
  end_loop
end

;eof wheel_translation.dvr

xvi. Wheel_rotation.dvr

;fname wheel_rotation.dvr

define wheel_a_acc ;Constant angular acceleration
  wheel_a_vel=wheel_alpha*(rot_time)
  wheel_kph=wheel_a_vel*wheel_avg_rad*3.6
  loop nn (1,num_wheel_walls)
    w_rvel(wheel_add(nn))=wheel_a_vel
  end_loop
end

define w_bearing_mom
  wbm=-100*wheel_a_vel
  if wbm>w_b_mom_max
    wbm=w_b_mom_max
  endif
  if wbm<-w_b_mom_max
    wbm=-w_b_mom_max
  endif
  w_bearing_mom=wbm
define wheel_Newton_rot ;Free rotation

wall_mom=0
loop nn (1,num_wheel_walls)
  wall_mom=wall_mom+w_mom(wheel_add(nn))
end_loop

wheel_AA=(wall_mom+w_bearing_mom)/Ig
wheel_a_vel=wheel_a_vel+wheel_AA*tdel
wheel_kph=wheel_a_vel*wheel_avg_rad*3.6

loop nn (1,num_wheel_walls)
  w_rvel(wheel_add(nn))=wheel_a_vel
end_loop

end ;eof wheel_rotation.dvr

xvii. Check_pt_solve2.fis

;performs solve command repeatedly with periodic breaks for checkpoint saving
;the 'comment' variable is a string describing the current phase. It is displayed during
cycling to allow easy recognition of simulation progress

def ck_pt_solve2
  ck_pt_run=ck_pt_run+1 ;tracks which instance of solve command is being manipulated
  ck_pt_complete=0 ;tracks whether crash occurred during or between solves
  equil_cntr=0
  done=0
  loop while done=0
    command
      print comment
      solve ave ck_pt_ave max ck_pt_max time ck_pt_time clock ck_pt_clock fish wheel_speed
      save fname2
    end_command
    done=1 ;default
    if av_unbal/av_cforce<ck_pt_ave
      else
        if max_unbal/max_cforce<ck_pt_max
          else
            if time>ck_pt_time
              else
                if wheel_speed=1
                  else
                    done=0 ;because termination of SOLVE was due to timeout for checkpointing
                  end_if
                end_if
              end_if
            end_if
          end_if
        end_if
      end_if
    end_if
  end_loop
  ck_pt_complete=1
end
ck_pt_run=0
REFERENCES


